

Molecular Dynamics News

number 99, February 1999

MDN is an informal newsletter of coming attractions and current events in the world of reaction dynamics and associated phenomena. It is produced without profit through the support of its subscribers* and patrons. Please renew your subscription by using the form at the bottom of this page.

The format for MDN is

- a Announcements of *open positions* (faculty and postdoctoral).
- b Information about *papers*, whether accepted or not, which are available for distribution. Please state in separate lines: *Title. Journal* (If ms. has been accepted - otherwise state *unpublished*). *Author(s). Address.* (Star author to whom correspondence should be addressed and whose mailing address is given.) In a separate final line provide a *one-sentence punch line*. Please follow this format.
- c Announcements of *conferences, topical meetings, etc.* Availability of *special materials* (e.g., annual reports, computer programs, experimental designs and tips, etc.). *Progress* (or activity) *reports* about work which is not yet published but which may be of interest to our community.
- d Electronic mail addresses and FAX numbers.

MDN is edited by Prof. Vincenzo Aquilanti, Dipartimento di Chimica dell' Università, 06123 Perugia, Italy (electronic mail: AQUILA@DYN.UNIPG.IT)

and Prof. Roger W. Anderson, Dept. of Chemistry, University of California, Santa Cruz, CA 95064, U.S.A. (electronic mail: ANDERSO@CATS.UCSC.EDU).

Send all material for issue 100 to Prof. R. Anderson (**You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU**). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#99). The closing date for issue number 100 is April 1, 1999.

*1999 Calendar-Year subscription for MDN, (six issues).

North America: (\$20/year US currency) : Your check for one or more years should be paid out to The Regents of the University of California. Send it to Roger W. Anderson, and include your name, address, and optional information like email addresses and FAX numbers.

Elsewhere: Your check for the equivalent of US \$20/year in any convertible currency should be paid out and sent to Prof. V. Aquilanti. **Amount enclosed**

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ANNOUNCING ELECTRONIC DELIVERY OF MDN

We offer to our subscribers several possibilities for electronic delivery of MDN:

1. Electronic mail to subscribers

In this case subscribers tell us if they want the newsletter automatically sent to them by electronic mail. The newsletter can be sent in two forms: raw LaTeX source file, or as a Postscript file. Subscribers may specify the desired form.

2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file. A Web browser such as Mosaic or Netscape with suitable viewers allows people to read the files on their computer screens. Alternatively the files can be downloaded for local viewing or printing. Subscribers choosing this delivery option will receive an email announcement when a new issue is posted. For information you are welcome to visit the Molecular Dynamics News World Wide Web site:

<http://www.ucsc.edu/mdn>

We periodically update the home page, and you can find links to Molecular Dynamics News subscribers' home pages at our WWW site. We will add a link to your home page if you send us the address by email or with the subscription form on the cover page of this issue. There is also a list of MDN subscribers that is linked to their email addresses. We appreciate electronic mail with your reactions to this proposal and with updated email addresses. Please send your email messages to MDN@CHEMISTRY.UCSC.EDU We continue to send hardcopy newsletters by mail to subscribers who request this form of delivery.

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

All members of the chemical physics community are invited to join the (free) "molecular-dynamics-news" email list. The "molecular dynamics" in the title is to be interpreted as meaning "dynamical processes in molecules" rather than "classical simulations of molecular motion". The list can be used to distribute details of conferences, vacant academic and postdoctoral positions, changes of address and other news in the Molecular Dynamics field. It also serves as an archive of up-to-date email addresses for people in the field. The list was created by Jeremy Hutson in June 1993 and has now about 1300 members.

Instead of being maintained manually, the list is operated by a system called "mailbase". People can join or leave the list simply by sending messages to the mailbase program, without the list owner needing to do anything. To join the email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

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join molecular-dynamics-news John F Kennedy
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You do not need to tell the program your email address, as it picks it up from the message header. It does need to be told your real name, so that it can maintain a useful list of email addresses.

When you join, you will receive some introductory information on how to circulate information to the molecular-dynamics-news list, and on the mailbase system itself.

If you would like a list of the current members, send a message containing the line
review molecular-dynamics-news

to the address mailbase@mailbase.ac.uk

Note that messages distributed via the e-mail list are not normally printed in the newsletter, unless the Editors receive an explicit request to do so.

There is also a spectroscopy email list. To join this email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

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join spectroscopy-group John Kennedy
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a. Open Positions

FACULTY

UNIVERSITY OF DURHAM

LECTURESHIP IN PHYSICAL CHEMISTRY (VACANCY REF. A038D)

The Department of Chemistry seeks a Lecturer (Grade A) with teaching and research skills in experimental physical chemistry. The appointment is for three years from 1 September 1999 in the first instance and may be extended for two further years. The successful candidate will have a Ph.D. and a track record of research as well as a strong interest in teaching. He or she must demonstrate ability to undertake independent research. Details of the Department (with current research interests) are to be found on <http://www.dur.ac.uk/~dch0www/> and further particulars of the post and an application form may be obtained from the Personnel Office. The salary will be in the range 16,655 - 21,815 pounds.

Formal applications, accompanied by a C.V. and the names of three referees should be sent in triplicate to the Personnel Office, Old Shire Hall, Durham, DH1 3HP, U.K. by 28 February 1999.

Please quote the reference number A038D in any enquiries.

Goteborg University

A position as Research Associate/Assistant Professor which is tenable for 2+2 years at the Department of Physics and Engineering Physics at Goteborg University, where a targeted area is modelling of reactions by classical and quantum molecular dynamics methods.

Closing date is 15 February 1999. More information is available in Nature no 6715, 14 Jan 1999, Classified 09.

Informal information can also be obtained from

Gunnar Nyman via email: nyman@phc.chalmers.se

Gunnar Nyman Office ph.: +46-31-7722270 Department of Chemistry, Secretary: +46-31-7722830 Physical Chemistry, Fax: +46-31-167194 Goteborg University, S-412 96 Goteborg, Sweden

University of East Anglia, Norwich, England

Five new full time academic appointments are to be made in the School of Chemical Sciences at the University of East Anglia, Norwich, England. One of the appointments (number 4 in the list below) is likely to be in the area of Laser chemistry, with particular reference to applications in environmental science. Informal enquiries concerning this post can be made to the author (s.meech@uea.ac.uk) or Prof. David Andrews (d.l.andrews@uea.ac.uk, 01603 592005) Details of the advertisement follow. It is hoped to conduct interviews between the 25 Jan and 5th Feb.

The University has recently announced a substantial investment in the School of Chemical Sciences, enabling it to strengthen core chemistry and to increase its interdisciplinary links with the Schools of Biological and Environmental Sciences, and also with the major science Institutes of the Norwich Research Park.

Accordingly, the School of Chemical Sciences now seeks to build further research strengths in major areas of chemistry, to build further on its successful collaboration with the School of Biological Sciences, and to develop new initiatives with the School of Environmental Sciences. Five faculty posts are available as described below. Whilst it is expected that appointments will be made at lecturer or reader level, depending on the experience and academic record of the applicant, one of the appointments may be made at professorial level for an outstanding candidate. In the case of senior posts, candidates will be expected to provide academic leadership in research, and to further develop links between the School of Chemical Sciences and other UEA Science Schools, members of the Norwich Research Park and national and international research bodies.

Synthetic Organic Chemistry

Researchers with proven expertise in synthetic organic chemistry are welcome to apply. This post would be particularly suitable for those with interests in the synthesis of biomolecular targets such as carbohydrates, nucleic acids and proteins and the development of new synthetic methodology, such as combinatorial chemistry. Applicants seeking to develop collaboration within the Norwich Research Park, especially with

the School of Biological Sciences and with microbial and plant scientists in the John Innes Centre, or with food scientists in the Institute of Food Research, will be of particular interest.

Synthetic Inorganic Chemistry

Synthetic inorganic chemists, particularly those relevant to the newly-established Wolfson Laboratory for Environmentally Friendly Catalysis, are invited to apply. The purpose of this Laboratory is to develop and study homogeneous catalysts which avoid the use and production of environmentally harmful substances. Potential catalytic systems of current interest include metal-mediated free radical production, biphasic reactions, biomimetic redox cycling of metal, complexes in aqueous media, metal oxide and hydroxide nanoparticles and reactions in super-critical water.

Biological Chemistry

A protein chemist is sought with interests which will complement existing areas at UEA, such as metalloprotein biology and spectroscopy, and protein structure determination by NMR and X-ray crystallography. The successful candidate will further strengthen the already effective links between the Schools of Biological and Chemical Sciences or be able to exploit the biological strengths within the Norwich Research Park. Research interests in protein structure-function relationships, protein folding, intermolecular interactions or chemical enzymology are particularly welcome.

Physical/Environmental Chemistry

A physical chemist is sought with interests in the application of fundamental theory and/or laboratory techniques relevant to environmental chemistry. Preference may be given to candidates whose research will enhance existing strengths within the School of Chemical Sciences, and help build collaborative research and teaching programmes with the School of Environmental Sciences. Research strengths in the two Schools relevant to the post include: ultrafast laser spectroscopy, photophysics and photochemical kinetics; condensed phase dynamics; thermodynamics of non-ideal solutions.

Environmental Analytical Chemistry

Applications are invited for a post in Environmental Analytical Chemistry to strengthen research in Analytical Chemistry within the School of Chemical Sciences and to enhance links with the School of Environmental Sciences. The preferred applicant will develop novel measurement strategies and/or techniques for target analyte species of environmental relevance either in the hydrosphere or atmosphere. It is intended that the successful applicant will complement the current research interests of faculty at the Analytical interface in the Schools of Chemical and Environmental Sciences and, as appropriate, across the Norwich Research Park.

Stephen R. Meech, School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, UK e-mail: s.meech@uea.ac.uk, Tele.: 44 (0)1603 593141, Fax: 44 (0)1603 592003

The University of Nottingham

CHAIR IN COMPUTATIONAL and THEORETICAL CHEMISTRY Applications are invited from candidates demonstrating a high level of achievement in computational and/or theoretical chemistry and the leadership to establish a strong computational and theoretical chemistry group at Nottingham. The ability to develop links that underpin research in chemistry and at interdisciplinary interfaces, e.g. with materials engineering, pharmaceutical sciences or biological and medical sciences, will be important. Please quote ref. MCM/085.

Salary for the Chair post will be within the professorial scale, minimum 37,420 pounds per annum.

LECTURER IN COMPUTATIONAL and THEORETICAL CHEMISTRY Applications are invited for a Lectureship in Computational and Theoretical Chemistry. The successful candidate will be expected to develop collaboration with other research areas within the School. Please quote ref. LEG/428.

Salary for the Lecturer post will be within the range 16,655 - 29,048 pounds per annum, depending on qualifications and experience.

Further details and application forms are available from the Personnel Office, Highfield House, The University of Nottingham, University Park, Nottingham, NG7 2RD. Please quote relevant reference number. Fax: 0115 951 5205. Email: Personnel.Applications@Nottingham.ac.uk.

Tel: 0115 951 3260 - Chair posts. Closing date: 15 January 1999. Tel: 0115 951 5927 - Lecturer posts. Closing date: 12 February 1999.

<http://www.nottingham.ac.uk/Personnel/academic.htm#MCM/084&085>, <http://www.nottingham.ac.uk/>,
<http://www.nottingham.ac.uk/chemistry/new/>

The University of Manchester, UK, Chair of Physical Chemistry

Applications are invited for this professorial position, which is tenable in the Chemistry Department from 1st October 1999 or earlier, from candidates with outstanding research records in Physical Chemistry.

Applications from candidates with research interests in classical Physical Chemistry will be welcomed, but so will applications from cognate areas of other disciplines; the remit of the Chair will be interpreted flexibly. A Lectureship in Physical Chemistry may be available to support this appointment.

Informal enquiries may be made to Professor Colin Price, Head of Department of Chemistry (tel: 0161 275 4706; fax 0161 275 4273; email Colin.Price@man.ac.uk) or to Professor Gareth Morris (tel: 0161 275 4665; fax 0161 275 4598; email g.a.morris@man.ac.uk).

Application forms (returnable by 21 December 1998) and further particulars are available from the Office of the Director of Personnel, The University of Manchester, Manchester M13 9PL; tel: ++44 (0) 161 275 2028; fax: ++44 (0) 161 275 2221; email: personnel@man.ac.uk; web site <http://www.man.ac.uk>. Please quote the reference no. 828/98. As an equal opportunities employer, the University of Manchester welcomes applications from suitably qualified people from all sections of the community regardless of race, religion, gender or disability.

University of Utah

A full time Research Associate position is available in the DOE Accelerated Strategic Computing Initiative (ASCI) Center at the University of Utah. Salary will be \$60K per year with full benefits. The applicant must have a doctoral degree in a scientific discipline, in addition to experience in object oriented programming, including the use of C++, and experience with a Unix OS (SGI preferred) and scientific programming. Experience with FORTRAN programming, MPI parallelization, molecular dynamics, and/or electronic structure codes is desirable. The applicant must have the ability and desire to work in a high profile interdisciplinary environment.

A vitae, publication list, and three letters of recommendation should be sent to: Professor Gregory A. Voth, Director, Henry Eyring Center for Theoretical Chemistry, Department of Chemistry, University of Utah, 315 S. 1400 E. RM Dock, Salt Lake City, Utah 84112-0850, voth@chemistry.chem.utah.edu, (801) 581-4353 (fax), Web Site: <http://voth.chem.utah.edu/>

Howard University

Two or more positions at the Assistant Professor level are open in PHYSICAL and ANALYTICAL chemistry. Targeted areas include separations, surface, polymer, atmospheric and laser chemistry.

Applications should include a resume and a brief statement of proposed research. Send application and three letters of recommendation to Search Committee, Department of Chemistry, Howard University, Washington, DC 20059. Evaluation of applications will begin December 15, 1998 and continue until suitable candidates have been found. Outstanding applications in other areas will be considered. For further information about the department, see: <http://www.chem.howard.edu>

POST DOCTORAL AND VISITING

PDRA IN COMPUTATIONAL ANALYSIS OF WATER SPECTRA, University College London, Department of Physics and Astronomy

(Re-advertisement due to withdrawal of a candidate)

A postdoctoral research assistantship is available to start as soon as possible to work on an National Environmental Research Council funded project entitled 'Computational analysis of water absorptions at near infrared and optical wavelengths'. The project will involve the first principles computation of water vibration-rotation spectra using programs developed at UCL, analysis of laboratory spectra, estimation of total atmospheric absorption by water and the construction of a reliable database of water transitions.

The appointment will be at the lower end of the Research Staff Scale 1A, currently £15,735 - 23,651 per annum, depending on age, qualifications and experience plus £2,134 London weighting. The grant is for two years although it is College policy to appoint for one year in the first instance.

Candidates should have or be about to obtain a PhD in theoretical molecular physics/quantum chemistry, atmospheric physics/chemistry or a related discipline.

Prospective applicants are encouraged to make informal contact with Prof. Jonathan Tennyson (j.tennyson@ucl.ac.uk or 0171-380-7809). Applications should be in the form of a full curriculum vitae including the names and addresses of two referees and sent or emailed to

Prof. Jonathan Tennyson, Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom.

WWW: <http://www.tampa.phys.ucl.ac.uk/jonny>

POSTDOCTORAL POSITION, University of Toronto

Professor P. Brumer, Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 1A1.

Please call the attention of interested candidates to an open postdoctoral position in my research group. Our group is currently engaged in theoretical work on coherent control of molecular processes, light-matter interactions, semiclassical methods of propagation, quantum and classical analyses of laser induced intramolecular energy redistribution, classical-quantum correspondence, quantum chaos, and decoherence.

At present postdoctoral applicants are being sought to enhance our programs in coherent control and in quantum chaos. Interested applicants must be recent Ph.D. recipients and should have high quality training in either molecule-light interactions or quantum chaos/nonlinear dynamics.

Applicants are asked to send me their Curriculum Vitae, either via email (pbrumer@tikva.chem.utoronto.ca) or by regular mail at the above address. They should also arrange to have two or more letters of recommendation sent to me directly, either by email or by regular mail.

PHD STUDENTSHIPS, CHEMICAL DYNAMICS GROUP, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA, TAIWAN, ROC

PhD studentships are available in the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, ROC. The primary mission of the candidate is to investigate chemical dynamics of high energy carbon cluster C2 and C3 reactions with sulfur containing molecules and unsaturated hydrocarbons employing crossed molecular beams techniques. These reactions are relevant to the high temperature chemistry in outflows of dying carbon stars, combustion flames, and chemical vapor deposition processes. A second research option is to understand the reaction dynamics of CH and C2H radicals with unsaturated hydrocarbons as an important means to form highly unsaturated radicals in cold, interstellar molecular clouds. Candidates must have a masters degree or equivalent in physical chemistry or physics. Pertinacious energetic candidates should send inquiries to Dr. Ralf I. Kaiser, Institute of Atomic and Molecular Sciences, Academia Sinica, 1 Section 4, Roosevelt Rd., Taipei, 106, Taiwan, ROC. Tel:886-2-23645370; Fax:886-2-23620200; email:kaiser@po.iams.sinica.edu.tw. <http://po.iams.sinica.edu.tw/~kaiser>.

POSTDOCTORAL RESEARCH FELLOWSHIP, University of Coimbra

One or two postdoctoral research positions are available in Theoretical & Computational Chemistry at the Group of Professor A.J.C. Varandas. The position is for research on potential energy surfaces and reaction dynamics, including non-adiabatic effects. The emphasis will be on systems with relevance in atmospheric chemistry and combustion processes. Applicants are sought with good experience on *ab initio* electronic structure calculations and/or reaction dynamics. The position is initially for one year, with renewal depending on mutual agreement. Applicants are welcome from all nationals who have obtained a PhD, with the position being available at the earliest convenience. Interested candidates should submit a curriculum vitae, and arrange for two or three letters of recommendation to be sent to:

Professor A.J.C. Varandas
Departamento de Química
Universidade de Coimbra

3049 Coimbra Codex, Portugal

For further information please contact Professor A.J.C. Varandas via e-mail: VARANDAS@QTVS1.UC.PT; telephone: 351-39-835867; fax: 351-39- 827703

POSTDOCTORAL POSITION, Lawrence Livermore National Laboratory

A postdoctoral position currently exists at the Energetic Materials Center, Lawrence Livermore National Laboratory. We are looking for a candidate to participate in a new effort to develop mesoscale models and apply simulations of large heterogeneous energetic materials. The candidate should have a Ph.D in Physics, Chemistry, Materials Science, or a closely related field, and should have a solid background in molecular/classical dynamics. The position offers excellent interaction with scientists from different fields and a state of the art computational facility. Interested parties should forward: 1) a c.v., 2) a publication list, and 3) the name and addresses of three references, to :

Dr. M. Riad Manaa Lawrence Livermore National Laboratory P. O. Box 808, L-282 Livermore, CA 94551 or via email to: manaa1@llnl.gov (i.e. MANAA1@LLNL.GOV)

Postdoctoral Position in Spectroscopy, Royal Institute of Technology, Stockholm

A 2-year Postdoctoral position at KTH (Royal Institute of Technology) within the framework of a DARPA-financed project at FOA (Swedish National Defence Research Establishment) is available. Knowledge of experimental methods in molecular spectroscopy and chemical physics, as well as the capability of handling pulsed lasers and various spectrometer systems are required. The existing and planned experimental facilities consist of different types of discharge sources, a closed-cycle cryostat equipment and different types of lasers. The capability of planning, setting up and running new experimental equipment is a requirement. Programming experience, as well as knowledge of matrix isolation techniques are appreciated. Location: FOA 2, Grindsjn (50 km outside Stockholm) Duration: 2 years. Salary: 25000 SEK/month Contact person at FOA2: Dr Olli Launila. Tel +468/7064098 or 7064068 Fax +468/7063949 E-mail olli@sto.foa.se

Contact person at KTH: Dr Lars-Erik Berg. E-mail: berg@atom.kth.se
<http://www.atom.kth.se/~berg/foa.html>

Applications should be sent (before April 15, 1999) to: Dr Olli Launila FOA2 Grindsjn SE-147 25 Tumba Doc Lars-Erik Berg, Studierektor, Fysik, KTH, Atom och Molekylfysik, Tel 08-790 7124, Institutionen fr Fysik, FAX 08-20 04 30, Lindstedsv.24, e-mail: berg@atom.kth.se, 100 44 Stockholm, <http://www.atom.kth.se>

POST DOCTORAL POSITION, UNIVERSITY OF BORDEAUX, FR

A post-doctoral position, funded by the European Commission under the TMR network "Astrophysical Chemistry" programme, is available for one or two years in our laboratory. The network involves eight research groups performing high level, experimental, theoretical kinetics and dynamics, and astrophysical modelling: U. of Birmingham (GB), Chemnitz (DE), Goettingen (DE), Perugia (IT), Rennes (FR), Bordeaux (FR), U.C. London (GB) and the Observatory of Meudon (FR). The focus for the following project is on experimental work, but interest in theory, strongly developed in the laboratory, is suitable. Reactions of C and Si atoms with small molecules will be investigated with combined pulsed lasers and pulsed, crossed, supersonic molecular beams. The crossed beam machine recently developed allows for scanning the kinetic energy of colliding partners down to values (0.4 kJ/mol) relevant to the conditions of the interstellar medium (see C.R. Acad. Sci. Paris Serie IIc., 1998, 771). Annual net salary will be around 23000 Euros. The postdoc associate will also have funds to spend up to one month per year of appointment in another laboratory of the network in order to complete his training. Interested candidates who fulfill the eligibility conditions required for TMR network young visiting researchers (see <http://www.cordis.lu/tmr/src/elcond.htm>) should submit a CV and the names of one or two referees to: Dr Michel Costes UMR 5803 CNRS - Universite Bordeaux I Laboratoire de Physico-Chimie Moleculaire Universite Bordeaux I 33405 Talence cedex, France phone: 33 5 56 84 63 45 fax: 33 5 56 84 66 45 email: costes@cribx1.u-bordeaux.fr

POSTDOCTORAL POSITION IN MOLECULAR LASER SPECTROSCOPY, Mississippi State

University

A postdoctoral research associate position will be available in molecular laser spectroscopy at Mississippi State University's Diagnostic Instrumentation & Analysis Laboratory (DIAL). DIAL is a multidisciplinary research and development institute, funded predominantly by the Department of Energy. The major emphasis of our research programs concerns application of modern instrumentation including lasers to environmental, combustion and propulsion problems. Many of the projects have both basic and applied aspects.

The research associate for this project will work on application of laser spectroscopy (especially cavity ring-down spectroscopy, photoionization/time-of-flight mass-spectrometry, and laser-induced fluorescence) to environmental/combustion problems. He/she should have a strong background (publications) in laser spectroscopy or a related area.

The associate can expect a salary of ~\$30-32K per year, plus medical insurance and moving expenses.

Interested individuals with appropriate research background should promptly send a cover letter and a CV (preferably by e-mail or fax) and have 2-3 recommendation letters sent directly to: Dr. R.Vasudev, Mississippi State University, Diagnostic Instrumentation & Analysis Laboratory, 205 Research Boulevard, Research & Technology Park, Starkville, MS 39759-9734; Fax:(601)-325-8465; E-mail: vasudev@dial.msstate.edu.

Individuals who had responded to an earlier advertisement need not reapply because their applications are on file.

We are an equal opportunity, affirmative action institution.

Ram Vasudev Mississippi State University 205 Research Boulevard, Research & Technology Park Starkville, MS 39759-9734, USA Phone: (601)-325-0499 (Office); (601)-325-9039 (Lab) Fax: (601)-325-8465 E-mail: vasudev@dial.msstate.edu

POSTDOCTORAL POSITION, University of Nevada

A postdoctoral position is available for a Ph.D. in Chemistry or Chemical Physics or related area for experimental research in gas phase ion-molecule reaction dynamics. Available projects, depending on experience and qualifications of the successful candidate, include (1) dynamics of SN2 reactions, (2) proton transfer and hydrogen atom transfer reactions of hydrocarbon anions, and (3) transition metal cluster reactivity and photodissociation dynamics. Additional information about the research program is available at <http://www.chem.unr.edu/faculty/kme>.

Applications including a vita, summary of research experience, and names of three references should be sent to Dr. Kent M. Ervin, Department of Chemistry/216, University of Nevada, Reno, NV 89557, and received by March 1, 1999, to assure full consideration. Minimum salary \$28,000 + benefits; Term: one year, renewable with mutual consent and continued funding. The University of Nevada, Reno, is an Affirmative Action/Equal Opportunity employer.

Kent M. Ervin Phone: 775-784-6676 Department of Chemistry/216 FAX: 775-784-6804 University of Nevada E-mail: ervin@chem.unr.edu Reno, NV 89557 Web sites: <http://www.chem.unr.edu> (Chemistry) <http://www.chemphys.unr.edu> (Chemical Physics) <http://beamer.chem.unr.edu> (Ervin Group)

POSTDOCTORAL POSITION ON SINGLE MOLECULE FLUORESCENCE MICROSCOPY, University of Cambridge

A three year postdoctoral position is available immediately at the University of Cambridge, Department of Chemistry under the supervision of Dr David Klenerman and Dr Shankar Balasubramanian. The project is to perform single molecule fluorescence spectroscopy on cryofixed biomolecules (rapidly frozen in water) in order to determine the relative stability of different conformations by studying individual molecules labelled with suitable fluorophors. The apparatus for cryofixation, the cold stage for the microscope and the single molecule fluorescence microscope have all been built. We are looking for someone with a background in laser spectroscopy and optics. No knowledge of molecular biology is required but an interest to learn about this subject would be useful. We are seeking to recruit some-one as soon as possible. To apply please send a CV and the name of two referees to:

Dr David Klenerman Department of Chemistry Lensfield Road Cambridge CB2 1 EW
fax:44-(0)1223- 336362 email: dk10012@cam.ac.uk

POSTDOCTORAL POSITION, SCHOOL OF CHEMICAL SCIENCES, UNIVERSITY OF EAST ANGLIA

Bioimaging with Ultrafast Lasers

Applicants are invited to develop two-photon fluorescence bioimaging of biological materials. The project, funded under the BBSRC Initiative on Bioimaging, is an interdisciplinary collaboration between the Ultrafast Laser and the Metalloprotein Groups in the School of Chemical Sciences and the Cell Biology Department of the John Innes Centre for Plant and Microbial Science, Norwich. The successful candidate will be based in the Ultrafast Laser group and will be responsible for the operation of an amplified titanium sapphire laser system, and associated optical instruments for multiphoton spectroscopy and imaging. A candidate is sought with experience of one or (preferably) more of the following: ultrafast lasers; nonlinear optics; imaging optics.

The post is available immediately for a period of three years

Salary will be in the RA1A range (£ 15,753 - £ 23651 per annum)

Applicants should send a CV including the names of two referees to Dr S. R. Meech, School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, UK. (e-mail: s.meech@uea.ac.uk, tel: 01603 593141, FAX: 01603 592003

Postdoc position in theoretical chemistry, Darmstadt University

A postdoctoral position is available at the chemistry department of the Darmstadt University of Technology in the group of Prof. Dr. J. Brickmann. The position is part of the Graduiertenkolleg "Kinetics and Mechanisms of Ionic Reactions" and can be occupied at April 1st, 1999 for a limited time (3 years). Prerequisites are experiences in theoretical chemistry, preferably in the field of computer simulations of complex systems, and in the application of standard program packages molecular dynamics (Monte Carlo, ab initio, Car Parrinello).

The field of research should be along the lines of the Graduiertenkolleg and it is expected that the applicant will participate actively in the GK. Also, the applicant should support various experimental groups with theoretical calculations within the GK. The scholarship follows the guidelines of the Deutsche Forschung for Graduiertenkollegs.

Applicants should send their CV, publication list, and names of two references to:

Speaker of the Graduiertenkolleg Prof. Dr. K.-P. Dinse Technische Universitt Darmstadt Petersenstr. 20 D-64287 Darmstadt Germany

Postdoctoral Position in Atmospheric Chemical Kinetics, University of Michigan

A postdoctoral position is available immediately for laboratory studies of free radical reaction kinetics in the aqueous phase. The work is motivated by the need for accurate free radical reaction mechanisms and rate constants in atmospheric chemistry models; "halogen activation" via free radical mechanisms will be a major theme. A second major theme will be the investigation of ionic strength effects. The position has funding for two years. A strong background in experimental chemical kinetics is required. Applicants should send a CV and publication list, a letter describing research interests, and the names of two, or three references to Prof. John R. Barker (jrbarker@umich.edu); Department of Atmospheric, Oceanic, and Space Sciences; The University of Michigan; Ann Arbor, MI 48109-2143.

John R. Barker Department of Atmospheric, Oceanic, & Space Sciences & Department of Chemistry 1520 Space Research Building University of Michigan Tel: 734-763-6239 2455 Hayward Street Fax: 734-764-5137 Ann Arbor, MI 48109-2143 (USA) jrbarker@umich.edu

POSTDOCTORAL APPOINTMENT, Argonne National Laboratory

A post-doctoral position in the Chemical Dynamics Group at Argonne National Laboratory with Albert Wagner and Michael Davis is open. The research involves the development of techniques for reducing the dimensionality of complex chemical kinetics and the incorporation of these reductions into computational fluid dynamics codes describing reactive flows. Of particular interest is the application of low-dimensional manifold techniques for this reduction, but other reduction approaches may also be explored. The project as it has developed is interdisciplinary, involving work in numerical analysis, applied mathematics (particularly

dynamical systems), theoretical chemistry, and kinetic modeling. The successful candidate should have some experience in one of these areas.

The Chemical Dynamics Program at Argonne consists of ten permanent staff members, five theoreticians and five experimentalists. It offers a unique opportunity for the close interaction between theory and experiment.

The group has a leadership role in a network of groups at Argonne that have a common interest in the simulation of combustion systems. The postdoctoral appointment will carry out research in the context of this network. In this regard, joint projects with computational fluid dynamicists from other groups involved in direct numerical simulation of combustion processes may arise during the course of this appointment.

Argonne is a National Laboratory operated by the University of Chicago for the Department of Energy, and is an equal opportunity employer. The laboratory is located about 25 miles west of Chicago.

The position is available immediately. Applicants must have received their Ph.D. no later than three years before their starting date. Please send a c.v. and have two letters of recommendation to Albert Wagner or Michael Davis, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439

Any of this information, and any questions, can also be mailed electronically to wagner@tcg.anl.gov and davis@tcg.anl.gov or faxed to 630-252-4470

POSTDOCTORAL POSITION, University of Birmingham

A 2-year PDRA funded by EPSRC is available from July 1999 to develop multi-channel CCD fluorescence detectors to cover the range ca. 100-700 nm for use at the Daresbury Synchrotron Radiation Source. These detectors will be used to record dispersed emission spectra over this wavelength range, following photoexcitation of species either in the gas phase, in clusters, or in the solid state by vacuum-UV or soft-X-ray radiation from the Daresbury SRS. The successful candidate will participate in experiments using these detectors of Dr R P Tuckett (Birmingham), Dr J C Whitehead (Manchester) and Prof B Hamilton (UMIST). A background in some branch of chemical physics is required, ideally with experience of optics and fluorescence detection. Previous experience of synchrotron radiation is not necessary. Initial salary in the range 15735-17570 UK pounds p.a. Applications, to include the names and addresses of two referees, to Dr R P Tuckett, School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT [tel 0121 414 4425, fax 0121 414 4403, email r.p.tuckett@bham.ac.uk] by 22 March, 1999.

Applications are also invited for two 3-year Research Studentships, available from September 1999, to join a collaboration between the groups of Drs R P Tuckett (Chemistry, Birmingham) and P A Hatherly (Physics, Reading). This new project, recently funded by EPSRC, is titled : 'Vacuum-UV photodissociation and photoionisation spectroscopy of gas-phase polyatomic molecules'. One student will be registered for a PhD at each University, but many of the experiments are synchrotron-based and will be performed at either the Daresbury or the BESSY, Berlin source. The experimental techniques used include fluorescence-excitation and coincidence spectroscopies. Details can be found in two recent papers, J. Chem. Phys. (1998) 108 857-868 and Zeit. Phys. Chem. (1996) 195 97-136. Candidates either holding or hoping to gain a 1st or upper 2nd Honours degree this summer (or those with an MSc degree) are asked to write to either Dr R P Tuckett (details above) or Dr P A Hatherly, Department of Physics, University of Reading, Whiteknights, Reading RG6 2AF [tel 01189 318578, fax 01189 750203, email p.a.hatherly@reading.ac.uk] also by 22 March, 1999.

Dr Richard P Tuckett, School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT , UK Tel : 0121 414 4425 / 4423 (messages) Fax : 0121 414 4426 Email : r.p.tuckett@bham.ac.uk Web : http://www.che.bham.ac.uk/research_labs/tuckett.html

POSTDOCTORAL POSITION, University of Waterloo

There is an immediate opening for a post-doctoral fellow in the area of tropospheric modelling in the Atmospheric Research Group at the University of Waterloo.

This position is part of a collaborative project involving industry, government and university researchers. While the position is located primarily at the University of Waterloo, the candidate will work closely with all of the partners, and will spend some time in each of the participating organizations. Applicants should have experience in atmospheric chemistry as well as some familiarity with tropospheric dynamics and with large-scale computing techniques.

The Atmospheric Research Group at the University of Waterloo is a collaboration between Prof. J. Pawliszyn and Prof. J.J. Sloan. Presently, it is focused on the development of new monitoring techniques for tropospheric gas phase and particulate pollutants, with a strong emphasis on urban and indoor air quality. The successful candidate will lead the expansion of this group into the area of modelling. There will be substantial assistance from our collaborators in government and private industry with this effort. Further information about related experimental projects in the Atmospheric Research Group may be found at our website: <http://www.science.uwaterloo.ca/chemistr/>, where the individual pages may be found at [pawliszyn.html](http://www.science.uwaterloo.ca/chemistr/pawliszyn.html) and [sloan.html](http://www.science.uwaterloo.ca/chemistr/sloan.html).

Applicants should forward a CV and two letters of reference to:

Prof. J.J. Sloan, Departments of Chemistry and Physics, University of Waterloo, Waterloo ON N2L 3G1, Tel: 1 519 888 4401, Fax: 1 519 746 0435, Canada. e-mail: sloanj@UWaterloo.CA, <http://www.science.uwaterloo.ca/chemistr/sloan.html>

POSTDOCTORAL POSITION, Weizmann Institute of Science, Israel

A postdoctoral position for a period of a year to two years is available in my group. Activities are focused on the theory of laser cooling of electronically excited polyatomic molecules, quantum thermodynamic rate theory, Laplace inversion methods, theory and control of surface diffusion. Recent publications are: P. Talkner, EP & A.M. Berezkhovskii, Binary collision theory for thermal and nonisothermal relaxation and reaction of polyatomic molecules, *Chem. Phys.*, Vol. 235, 131 (1998). G. Gershinsky and EP, Unimolecular reactions in the gas and liquid phases: A possible resolution to the puzzles of the trans-stilbene isomerization, *J. Chem. Phys.* Vol. 107, 812 (1997). EP and J.L. Liao, A new quantum transition state theory, *J. Chem. Phys.*, Vol. 108, 2733 (1998). J. Shao, J.L. Liao and EP, Quantum transition state theory: Perturbation expansion, *J. Chem. Phys.* Vol. 108, 9711 (1998). EP and B. Eckhardt, Semiclassical canonical rate theory, *Phys. Rev. E*, Vol. 58, 5436 (1998). J.L. Liao and EP, A test of quantum transition state theory for a system with two degrees of freedom, *J. Chem. Phys.* Vol. 110, p. 80 (1999). H. Wadi and EP, Accurate computation of quantum densities of states and RRKM rate constants for large polyatomic molecules - the STAIR method, *J. Chem. Phys.*, in press.

Work in the group involves both the development of analytic theory as well as numerical simulation for small and large systems. Previous experience with molecular dynamics and Monte Carlo methods is needed. Salary is ca. 22,000 USD per year, more than enough to cover living and housing expenses in Israel. Suitable candidates should send their cv's, list of publications and two letters of recommendation to Eli Pollak Chemical Physics Dept. Weizmann Institute of Science 76100 Rehovot, Israel Fax: +972 8 934 4123 email: cfpollak@weizmann.weizmann.ac.il

Ph. D. Studentship, UNIVERSITY OF YORK, DEPARTMENT OF CHEMISTRY

Applications are invited from UK/EU nationals for a Ph.D. studentship tenable from 1st October 1999 in the group of Dr. Martin Cockett to work

on ion-molecule reactions in cluster ions, studied using mass-resolved laser threshold ionisation techniques. Candidates should hold or expect to hold a first class or upper second class honours degree (or equivalent) in an appropriate discipline and have a strong interest in molecular spectroscopy (experience with lasers is not essential).

Further details of current research interests can be found at:

<http://www.york.ac.uk/depts/chem/staff/mcrc.html>

Interested candidates should in the first instance write, fax or email together with a CV to:

Dr. Martin Cockett Department of Chemistry University of York Heslington, York YO10 5DD UK
Tel: (01904) 434534 Fax: (01904) 432516 email: mcrc1@york.ac.uk

POSTDOCTORAL POSITION, National Taiwan University

A postdoctoral position is currently available in the Department of Chemistry, National Taiwan University, Taipei, Taiwan. The research will focus on one of the two topics: 1. photodissociation and photoionization of van der Waals molecules using a reflectron time-of-flight MS and 2. ion-molecule reactions using a new apparatus which is being constructed. Therefore, a candidate should have experience with pulsed molecular beam, laser technique, and mass spectrometer. The initial appointment will be for one year, but funds are

available for support more than one year. Applicants should send a CV and two letters of recommendation to Professor K. C. Lin, Dept. of Chemistry, National Taiwan University, Taipei, Taiwan 106, ROC. Tel: 886-2-23621483; Fax: 886-2-23621483; e-mail: kclin@mail.ch.ntu.edu.tw.

POSTDOCTORAL POSITION, National Tsing Hua University, Taiwan

Two postdoctoral positions starting 1999 (flexible) at the Department of Chemistry, National Tsing Hua University, TAIWAN. Possible projects include: (1) Two-color resonant four-wave mixing spectroscopy of free radicals in a supersonic jet, (2) Time-resolved Fourier-transform Spectroscopy with a step-scan FTIR - spectroscopy, kinetics, and dynamics after laser photolysis of gaseous molecules. (3) Photoionization spectroscopy and kinetic of free radicals using synchrotron radiation source or VUV laser. (4) Ultrafast phenomena - photodissociation and charge transfer mechanisms. Extended experiences with excimer and Nd-YAG lasers preferred. Good salary with yearly renewable appointment. Applicants should arrange 2-3 letters of recommendation to be sent to Prof. Y. P. Lee, I-C. Chen, Department of Chemistry, National Tsing Hua University, TAIWAN 300 (e-mail: yplee@net.nthu.edu.tw, icchen@net.nthu.edu.tw, FAX: 886-3-5722892)

POSTDOCTORAL POSITIONS, ETH, Zuerich

Two postdoctoral positions are open in the molecular kinetics and spectroscopy group of Martin Quack at ETH Zuerich for two new projects. The first project involves investigation of intramolecular primary processes on short (fs to ps) timescales (IVR and simple reactive processes such as stereomutation). In this project it is planned to study the same type of process by two techniques in parallel. 1. High resolution spectroscopy and fully time dependent quantum dynamics derived from this and 2. Femtosecond time resolved techniques. Whereas the first approach has been developed by our group over many years and the know how is available, new experiments are being built during for fs to ps time resolved spectroscopy. It would be useful for applicants to have experience with fs laser techniques.

The second project is situated in the framework of the alliance for global sustainability (AGS) and involves development of new high resolution (FTIR and laser) spectroscopic techniques for atmospheric spectroscopy. Applicants should be enthusiastic about these applications of spectroscopy, they should have adequate familiarity with high resolution spectroscopy, and should be willing to collaborate in an international framework. Both positions are available immediately for one year, renewable for one or more years upon mutual agreement. The salary is Sfr 60000.- per year (about 40000 USD). The positions would also be available to particularly gifted graduate students (the salary is then about 60 percent of the above amounts). Send applications to Prof. Martin Quack, Lab. for Physical Chemistry, ETH Zuerich (Zentrum), CH-8092 Zuerich, Switzerland.

Postdoctoral Positions, University of California, Berkeley

Two postdoctoral positions are available in the research group of Daniel Neumark at UC Berkeley. One position is in the field of molecular beam reaction dynamics. Research will focus on photodissociation and reactive scattering of hydrocarbon radicals using molecular beam instruments in my laboratory and at the Advanced Light Source. The second position is in the area of negative ion photoelectron spectroscopy. Research will be centered on studies of size-selected clusters, radicals, and transition states. A strong background in experimental chemical physics is required for both positions. Applicants should send their CV, publication list, and names of three references to: Professor Daniel Neumark, Department of Chemistry, University of California, Berkeley, CA 94720, USA

POSTDOCTORAL RESEARCH ASSOCIATE, University of North Carolina at Chapel Hill

Applications are invited for a one to two-year postdoctoral research position funded under the EPA STAR Grant project "Aerosol Partitioning and Heterogeneous Chemistry," in the research group of Dr. Roger Miller. The group's research focuses on investigating the chemical and physical properties of tropospheric and stratospheric aerosols.

The successful candidate will be involved in the development and implementation of an in situ spectroscopic technique for monitoring the composition and heterogeneous chemistry of tropospheric aerosols. This technique involves the combination of step-scan FTIR spectroscopy, tunable diode laser spectroscopy and

laser induced thermal desorption. The aerosols of interest include those currently being considered by the EPA as a component in future PM_{2.5} regulations. The goal is to develop non-invasive in situ methods for determining the properties of these semivolatile species.

Candidates are expected to have a PhD in chemistry, atmospheric science or related field. Experience with spectroscopy and lasers is necessary. Please send CV, a letter describing research interests and background, relevant publications and at least two letters of reference to Professor Roger E. Miller, Department of Chemistry, CB3290, Kenan Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3290, USA. Phone 919-962-0528, fax 919-962-2388, remiller@unc.edu.

POSTDOCTORAL APPOINTMENT, UNIVERSITY of OXFORD, UK

Applications are invited for a postdoctoral position in the Physical and Theoretical Chemistry Laboratory to work with M.S. Child on ab initio Rydberg dynamics. The aim is to combine an ab initio R matrix treatment of the electrons with the multichannel quantum defect approach to the nuclear motions, with a view to modelling ionization, dissociation and dissociative recombination processes. Knowledge of ab initio quantum chemistry and/or multichannel quantum defect theory is highly desirable. The tenure of the appointment is for up to two years on a salary scale between 17570 and 20107 GBP pa, according to age and experience. Applications including a cv and contact details for two academic referees should be sent to Prof M.S. Child, Physical and Theoretical Chemistry Laboratory, South Parks Rd, Oxford OX1 3QZ, UK. Fax +44 1865 275410 (see <http://physchem.ox.ac.uk/msc/> for further details)

POST-DOCTORAL POSITIONS, University of California, Berkeley

Opportunities are available on the new Chemical Dynamics Beamline at the Advanced Light Source to study reaction dynamics and photochemistry of radicals and clusters. This unique User Facility (<http://www.lbl.gov/chemicaldynamics>) features a 10cm undulator providing 1e16 VUV photons/second continuously tunable from 5 to 30 eV, along with dedicated molecular beam endstations using both neutral time-of-flight as well as ion imaging detection methods in addition to extensive laser resources.

Successful candidates will be expected to develop new radical and cluster molecular beam sources; perform studies of radical photochemistry, crossed-beam reaction dynamics or cluster spectroscopy and dynamics; develop innovative applications of synchrotron radiation to chemical dynamics studies such as coincidence imaging studies of neutral photochemistry; perform collaborative studies with outside users; publish results in recognized journals.

These positions require a PhD in Chemical Physics or a related discipline, experience in molecular beam photochemistry or reaction dynamics studies and a record of publication in chemical dynamics or a closely related field. Experience with synchrotron radiation is useful but not necessary.

Interested applicants should send a CV and arrange for two letters of recommendation (email preferred) to: Dr. Arthur G. Suits, Chemical Dynamics Group, MS 6-2100, 1 Cyclotron Road, E. O. Lawrence Berkeley National Laboratory, Berkeley CA 94720 USA, Tel +1 510-486-4754, Fax +1 510-486-5664, Internet agsuits@lbl.gov, <http://www.lbl.gov/~agsuits>

POSTDOCTORAL POSITION, Naval Research Laboratory, Washington, D.C.

Postdoctoral research positions in experimental physical chemistry are available for qualified candidates in the Chemistry Division at the Naval Research Laboratory, Washington, D.C. The opportunity is for femtosecond laser studies of molecular dynamics, such as energy transfer and photodissociation. Projects include studies of molecules in gases, liquids and on interfaces. Applicants familiar with ultrafast lasers and molecular dynamics are preferred. Fellowships are awarded through the NRC, and appointments are for a minimum of one year, renewable to two years. The annual stipend is \$48,000. Information on our research, including a publication list, and links to the NRC Postdoctoral Program can be found on our webpage, <http://chem1.nrl.navy.mil/molecular>

For more information, please contact: Jeff Owrutsky, Code 6111, Naval Research Laboratory, Washington, D.C. 20375-5342, (202)-404-6352 [voice], jeff@chem1.nrl.navy.mil (U.S. Citizens only.)

Postdoctoral Research Position in Surface Probe Microscopy

Our group is interested in chemical and physical processes at solid/liquid interfaces. The laboratory is well

equipped with STM/AFM, in addition to nsec, psec, and fsec lasers for linear and nonlinear optical laser experiments. Our work is supported by NSF, DOE, and Research Corporation.

The objective of the current project is to study interface dynamics and will ultimately involve combining SPM and optical probes. This is a good opportunity for an individual with strong SPM skills seeking to learn more about optical probes of interfaces. Candidates should have previous experience with STM/AFM. Experience with lasers is a plus. The candidate should have strong problem solving skills, work well with others and demonstrate scientific leadership and initiative.

The Surface Science Center at the University of Pittsburgh provides an excellent research environment. The city of Pittsburgh is safe, pleasant and affordable.

The position is for one year, with possibility of renewal. Applicants should submit a curriculum vitae, a list of publications, a reprint of their most significant work, a statement of research interests and objectives, as well as names and addresses of three references who are willing to write letters of recommendation.

Dr. Eric BORGUET, Department of Chemistry and Surface Science Center, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh PA 15260, (412) 624-8304 Office, (412) 624-8305 Lab, (412) 624-8611 Fax, borguet+@pitt.edu, <http://www.chem.pitt.edu/faculty/borguet.html>

POSTDOCTORAL POSITION, VRIJE UNIVERSITEIT, AMSTERDAM

In the ACAS (Analytical Chemistry and Applied Spectroscopy) department of the Chemistry Division, Faculty of Sciences, a two-year postdoctoral position is available in laser spectroscopy. In this department a new line of experimental physical-chemistry research is initiated in the field of dynamic processes in the condensed phase, using an advanced lasersystem, in a newly built laserlab. The aim of this research is to obtain insight in excitation transport and excitation relaxation in complex systems, such as porphyrin clusters and films, and porphyrin-protein complexes. The successful candidate will be expected to perform time-resolved resonance Raman and fluorescence spectroscopy on condensed phase systems, on a pico to nanosecond time scale, as part of the program "Spectroscopy and Dynamics of Complex Systems", and to (co)-supervise graduate and undergraduate students in this project. A contribution to the teaching activities of ACAS is also expected. Applicants should have a PhD in physical chemistry, and have practical experience in the field of time resolved laser spectroscopy. Demonstrated interest in (bio)-physical systems would be an advantage.

Further information may be obtained from Prof. Dr. C. Gooijer, (31-20-4447540) or Dr. G. van der Zwan (31-20-4447635, zwan@chem.vu.nl, FAX: 31-20-7643). Applications, including a curriculum vitae, should be addressed to Drs. G. Veerbeek, Faculty of Sciences, de Boelelaan 1081 a, 1081 HV, Amsterdam.

POSTDOCTORAL POSITION, UNIVERSITY COLLEGE, LONDON

A three-year EPSRC funded Postdoctoral Research Assistantship in Theoretical Molecular Physics is available. The post is to work with Prof Jonathan Tennyson and Dr Lesley Morgan on low-energy electron-molecule collisions using the R-matrix method. The project would suit a candidate with a background in either atomic and molecular physics or quantum chemistry. The appointment would be on the lower part of the Research Staff Scale 1A, currently £ 15,735 –£ 22,785 p.a. plus £ 2134 London weighting.

Further information can be obtained from: Jonathan Tennyson, Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK, Tel: +(44) 171 380 7809, Fax: +(44) 171 380 7145, Email: j.tennyson@ucl.ac.uk, WWW: <http://www.tampa.phys.ucl.ac.uk/jonny>

Applicants should send a curriculum vitae, including the names of two referees, as soon as possible to Prof Jonathan Tennyson.

POSTDOCTORAL POSITION, Michigan State University

A postdoctoral position is available in the general area of Femtosecond observation and control of chemical reactions in the research group of Marcos Dantus.

Because funding for this position will come from an Affirmative Action Postdoctoral Fellowship from the College of Natural Science at MSU candidates for the fellowship must be Black, Hispanic, Asian/Pacific Islander or Native American and must be U.S. Citizens or U.S. permanent residents.

This position includes a generous stipend and health coverage.

For information about our research group and about other opportunities visit our web page at:
www.cem.msu.edu/~dantus

For further information or to apply (C.V., and two letters of recommendation required) contact Professor Dantus directly at dantus@cem.msu.edu

Postdoctoral Position, Stanford University

A postdoctoral position is available in my research group at Stanford University in the area of semiconductor surface chemistry and semiconductor processing. The research will focus on in situ optical spectroscopic studies of chemical vapor deposition, chemical etching, and surface modification of group IV semiconductors. Techniques such as MIR-FTIR spectroscopy and REMPI are combined with mass spectrometry, scanning probe microscopy, and surface analytical techniques to investigate the reaction mechanisms, kinetics, and dynamics of these processes at the molecular level.

An enthusiastic, hardworking individual with a strong background in laser spectroscopy and/or surface science is preferred. The initial appointment will be for one year, with the option of a second year upon mutual agreement. The position is available immediately, but later dates may be arranged.

Applicants should submit a resume and have two letters of recommendation sent to Prof. Stacey Bent, Department of Chemical Engineering, 381 North-South Mall, Stanford University, Stanford, CA 94305-5025, or e-mail: stacey.bent@stanford.edu.

Stanford University is an equal opportunity / affirmative action employer encouraging applications from women and minority candidates.

Postdoctoral Position, University of Utah

A postdoctoral position is available immediately in the lab of Scott Anderson at the University of Utah. The experiment combines a flow tube reactor with a tandem guided ion beam mass spectrometer to study the unimolecular decomposition mechanisms of strained high-energy-density molecules (e.g. cubanes, quadricyclanes, bicyclobutanes). Ab initio calculations are carried out to aid interpretation. A secondary goal of the experiments is to test applications of low energy guided ion beam scattering to analytical mass spectrometry, and resolution of strained and chiral isomers will be investigated. More information on the instrument can be found in Int. J. Mass Spectrom. Ion Proc. 167/168 (1997) 269, or at the following web address: www.chem.utah.edu/chemistry/faculty/anderson/anderson.html. More information can be found in preprints, available upon request.

Experience with ion beams or mass spectrometry is helpful, however, the most important criterion is creativity. The initial appointment will be for one year, and is renewable for a second year based on progress and availability of funds. Salary will be competitive, and the position includes excellent health insurance. Salt Lake is a great place to live, with world-class skiing, hiking, and biking close by, good neighborhoods near campus, and excellent public schools. The University of Utah is an AA/EEO employer, and applications from qualified women and minority candidates is encouraged. If interested, please send a CV and arrange for three letters of recommendation to be sent to: Prof. Scott L. Anderson, Chemistry Dept., University of Utah, 315 S. 1400 E., Salt Lake City, UT 84112.

Prof. Scott L. Anderson, Chemistry Department, University of Utah, 315 S. 1400 E. RM Dock, Salt Lake City, UT 84112-0850, Ph:(801)585-7289, FAX:(801)581-8433, anderson@chemistry.utah.edu, <http://www.chem.utah.edu/chemistry/faculty/anderson/anderson.html>

POST-DOCTORAL AND RESEARCH FACULTY, University of California, San Diego

The Kent Wilson group, at the University of California, San Diego, Dept. of Chemistry and Biochemistry, has positions available for exceptionally talented experimental scientists in the following areas: ultrafast x-ray diffraction and absorption applied to chemical and biochemical dynamics and function, and new techniques in optical microscopy for spatially and temporally resolved imaging as applied to the understanding of dynamics of cellular and intercellular biomolecular and biological processes (including interneuronal communication and function). For more information about these positions and the group, or to receive application process information, visit our Web site, <http://www-wilson.ucsd.edu> OR email wgjobops@ucsd.edu. Positions commensurate with experience and qualifications, with salaries based on UC payscales.

POSTDOCTORAL POSITION, NAVAL RESEARCH LABORATORY

I am looking for a postdoctoral candidate in the Chemistry Division at the Naval Research Laboratory. These positions are administered by the National Research Council (NRC) and attract a nationwide pool of applicants. The candidate will work in a new research area measuring the fast kinetics of protein folding and conformational changes in synthetic biomaterials. I also intend to expand the program to low temperature measurements and begin to produce proteins and mutants of interest by recombinant DNA methods. The candidate's background should include at least two of the four areas: laser experience, infrared spectroscopy, a kinetics background, and knowledge of biological materials or systems. The instrumentation available in my laboratory includes: a Nd:YAG pulsed laser, a vacuum step-scan FTIR, a Raman shifter, a temperature programmed cell, a separate cold finger and chamber for low temperature experiments, and basic microbiology equipment. Other equipment for protein characterization, such as a CD spectrometer, UV spectrometers, and differential scanning calorimetry are available on site. This research opportunity and postdoctoral research program is described on the world wide web at

<http://dynamics-www.nrl.navy.mil/molecular/> and my web site is:

<http://dynamics-www.nrl.navy.mil/molecular/jane/jane.html>.

The postdoctoral candidates at the Naval Research Laboratory must be U.S. citizens. Initial appointments are for one year and are routinely renewable for a second year. The stipend is \$47,000 per year with additional funds for moving expenses and professional travel to meetings.

The applicant is responsible for selecting a research project and writing a short research proposal in collaboration with the prospective advisor. It is my experience that the application proposal takes about four weeks to complete. The deadlines for applications are 15 January 1999 and 15 April 1999, with the earliest possible starting times of July 1999 and October 1999, respectively. For further information please contact me through e-mail or by phone. Please post or share the attached announcement with your colleagues.

Dr. Jane K. Rice, Chemistry Division, Code 6111, Phone 202 767-0721, FAX 202 404 -8119,

Rice@ccf.nrl.navy.mil

POSTDOCTORAL POSITION, TEXAS TECH UNIVERSITY

I have a post-doctoral position available January 1, 1999, in my lab at Texas Texas Tech University. The research involves photoelectron spectroscopy of metal hydride anions, such as LiH_2^- , MgH_3^- , BH_4^- , and AlH_4^- . The desired candidate would have experience in laser spectroscopy, electronics, and computer programming. Experience with vacuum systems and mass spectrometry would also be helpful, but not required.

Applications, including a CV and 2 letters of recommendation, should be sent to:

Prof. Paul G. Wenthold, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409-1061, Ph (806) 742-3088, FAX (806) 742-1289, email: wenthold@dorothy.chem.ttu.edu

Texas Tech is an EE/AA employer.

POSTDOCTORAL POSITION, ARGONNE NATIONAL LABORATORY

A post-doctoral position is available in the Chemical Dynamics Group at Argonne National Laboratory. The research involves development and application of laser based experimental methods in high-temperature gas-phase kinetics in the laboratory of Jan P. Hessler. The successful candidate will be expected to measure the rates of reactions under non equilibrium conditions, perform state-to-state relaxation measurements, and study important dissociative and associative reactions. The results obtained from these experiments will be analyzed with state-of-the-art Master Equation and Monte Carlo techniques. The Chemistry Division of Argonne National Laboratory has a strong Chemical Dynamics Group, composed of several theoretical chemists and experimentalists, and the successful candidate will be encouraged to interact with others in the group and to develop new research ideas. The position is available immediately. However, depending upon circumstances, the successful candidate may choose to start in the coming Spring or Summer. Please send a curriculum vitae and have two letters of recommendation sent directly to Dr. Jan P. Hessler, Chemistry Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439-4831, Communication via electronic mail or facsimile to 1-630-252-4470 are acceptable.

POSTDOCTORAL POSITION, National Research Council of Canada

A postdoctoral position in theoretical chemical physics is available. The successful candidate will choose one (or more) of several planned research projects in the general fields of: (1) Molecular dynamics in intense and/or short-pulse laser fields (2) Reaction dynamics at interfaces (3) Mathematical method development. The starting date is flexible.

For more information about recent and ongoing research projects see

<http://gold.nrc.ca/~tamar>

For any other information please contact me at tamar@mahler.sims.nrc.ca or at Tel. 613-990-0945.

e-mail: tamar.seideman@nrc.ca, <http://gold.nrc.ca/~tamar>

Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Drive, Ottawa, Ontario K1A 0R6, Phone: (613) 990-0945, FAX : (613) 947-2838

POSTDOCTORAL APPOINTMENT, Argonne National Laboratory

The Gas Phase Chemical Dynamics Program at Argonne National Laboratory has an opening for a postdoctoral appointment working with R. Glen Macdonald. The research involves the use of high resolution time-resolved near infrared and infrared absorption spectroscopy to study the spectroscopy, dynamics and kinetics of radicals of interest to combustion and atmospheric chemistry. The main thrust of the program over the next few years will be to study the dynamics and kinetics of atom + radical and radical + radical processes; however, other studies are possible, depending on the qualifications and interests of the successful candidate. Several recent articles will give potential candidates an idea of the variety of problems that can be tackled with this apparatus; a) Infrared Spectroscopy, *J. Mol. Spectroscopy* 186, 349 (1997). b) Chemical Kinetics, *J. Phys. Chem.* 102, 4585 (1998), and c) Chemical Dynamics, *J. Chem. Phys.* 109, Sept. 15 (1998). The successful candidate should be planning to graduate soon or be a recent graduate from a Chemical Dynamics or Kinetics Program, and have experience in laser spectroscopy, vacuum techniques, and computer data acquisition. A background in rovibrational spectroscopy of polyatomic molecules would be a desirable asset. An application will require a CV and three letters of recommendation. For further information, interested candidates should contact Glen Macdonald.

The Gas Phase Chemical Dynamics Program at Argonne consists of ten permanent staff members, five theoreticians and five experimentalists. It offers an unique opportunity for the close interaction between theory and experiment. Argonne is a National Laboratory operated by the University of Chicago for the Department of Energy, and is an equal opportunity employer. The laboratory is located about 25 miles west of Chicago.

R. Glen Macdonald Ph. (630) 252-7742 Argonne National Laboratory Fax. (630) 252-4470 Chemistry Division Email. macdonald@anlchm.chm.anl.gov 9700 South Cass Ave. Argonne, IL 60439

POSTDOCTORAL POSITION, Hanscom Air Force Base A postdoctoral position for work in theoretical chemical dynamics is available at the Air Force Research Laboratory, Hanscom Air Force Base (about 10 miles north of Boston), MA. Successful candidates are expected to calculate cross sections for inelastic and reactive involving atom-molecule or molecule-molecule collisions. Position initially for one year - with a possibility for renewal for another year. Commensurate salary. U.S. citizenship or Green Card required. Reply to: sharma@plh.af.mil.

b. Preprints

Photodissociation of OCIO and Ar/OCIO and H₂O/OCIO clusters studied by the resonance enhanced multiphoton ionization-time of flight method

J. Chem. Phys.

C. J. Kreher, R. T. Carter and J. R. Huber*

Physical Chemistry Institute, University of Zurich, Wintherthurerstr. 190, CH-8057, Switzerland, carter@pci.unizh.ch

The effect of a cluster environment on OCIO dissociation was investigated by measurement of the internal excitation of the CIO photofragment and the O and CIO photofragment speed distributions.

Photodissociation of a surface-active species at a liquid surface: A study by time-of-flight spectroscopy

J. Phys. Chem.

Alan Furlan

Physikalisch-Chemisches Institut der Universitt Zrich, Winterthurerstrasse 190, 8057 Zrich, Switzerland.
furlan@pci.unizh.ch

Time-of-flight distributions of iodine fragments ejected from a liquid surface after a photoexcitation pulse indicate an accumulation and preferential orientation of the chromophores at the gas-liquid interface.

Two-frequency IR Laser Orientation of Polar Molecules-Numerical Simulations for HCN

Chem. Phys. Lett.

C.M.Dion, A.D.Bandrauk, A.Keller, O.Atabek, H.Umeda and Y.Fujimura

Laboratoire de Photophysique Moleculaire, Univ. Paris-Sud, Orsay, 91405, France; Graduate School of Science, Tohoku University, Sendai, Japan, 980.

Using ab-initio nuclear-coordinate dependent dipole moments and polarizabilities, the dynamics of "orientation" as compared to "alignment" was studied numerically by solving the corresponding full time-dependent Schroedinger equation in the presence of a superposition of intense, linearly polarized IR laser pulses of frequency ω and 2ω . Optimal orientation occurs for field configurations $E(t) = E_0(t) (\cos(\omega t) + 0.5\cos(2\omega t))$ where 2ω is resonant with a 0-1 vibrational transition for picosecond $E_0(t)$ pulses.

Charge Resonance Ionization of Molecular Ions in Intense Laser Pulses-Geometric and Orientation Effects.

Phys. Rev. A

A.D. Bandrauk and J. Ruel

Laboratoire de Chimie Theorique, Fac. des Sciences, Univ. de Sherbrooke, Que, J1K 2R1, Canada.

Numerical solutions of the time-dependent Schroedinger equation for one-electron 2-D H_2^+ , H_3^{++} molecular ions have been obtained in order to illustrate the dependence of Charge Resonance Enhanced Ionization, CREI, on the angular orientation of the molecule. For H_3^{++} both linear and triangular geometries have been considered. It is found in general that orientational effects on ionization rates, induced dipole moments and torques, are most significant at the critical distances R_c and critical angles θ_c of molecular geometry where CREI occurs. These exact calculations allow for estimation of the "alignment" times of the ions near the dissociative ionization regime of these ions in intense laser pulses.

Crossed-beam study of the $Al(^2P_{1/2,3/2}) + O_2$ reaction at low and very low kinetic energies unpublished

Christian Naulin and Michel Costes*

UMR 5803 CNRS - Universite Bordeaux I, Laboratoire de Physico-Chimie Moleculaire, Universite Bordeaux I, 33405 Talence Cedex, France

The reaction $Al(^2P_{1/2,3/2}) + O_2$ is revisited at low and very low kinetic energies (250 - 6 meV) with a new crossed beam apparatus.

Crossed-beam reaction of the cyanogen radical, $CN(X^2\Sigma^+)$, with acetylene, $C_2H_2(X^1\Sigma_g^+)$: observation of cyanoacetylene, $HCCCN(X^1\Sigma^+)$

J. Chem. Phys.

L.C.L. Huang, Y.T. Lee and R.I. Kaiser

Crossed-beam reaction of carbon atoms with hydrocarbon molecules V: chemical dynamics of n- C_4H_3 formation from reaction of $C(^3P_j)$ with allene, $H_2CCCH_2(X^1A_1)$

J. Chem. Phys.

R.I. Kaiser, A. Mebel, A.H.H. Chang, S.H. Lin and Y.T. Lee

Neutral-Neutral reactions in the interstellar medium II: isotope effects in the formation of l/c- C_3H and C_3D radicals in interstellar environments

Astrophys. J.

R.I. Kaiser, C. Ochsenfeld, M. Head-Gordon and Y.T. Lee

Crossed-beam reaction of carbon atoms with sulfur containing molecules I: chemical dynamics of

thioformyl (HCS; X^2A') formation from reaction of $C(^3P_j)$ with hydrogen sulfide, $H_2S(X^1A_1)$

J. Chem. Phys.

R.I. Kaiser, C. Ochsenfeld, M. Head-Gordon and Y.T. Lee

A Coupled-Cluster *ab initio* investigation of singlet/triplet CH_2S isomers and the reaction of atomic carbon with hydrogen sulfide to HCS/HSC

J. Chem. Phys.

C. Ochsenfeld, R.I. Kaiser, Y.T. Lee and M. Head-Gordon

Crossed beam reaction of atomic carbon, $C(^3P_j)$, with d6-benzene, $C_6D_6 (X^1A_1)$: observation of the per-deutero-1,2-didehydrocycloheptatrienyl radical, $C_7D_5 (X^2B_2)$

J. Chem. Phys.

R.I. Kaiser, I. Hahndorf, L.C.L. Huang, Y.T. Lee, H.F. Bettinger, P. v.R. Schleyer, H.F. Schaefer

The gas-phase fragmentation of trineopentylstannyl cation: a rare example of beta-methyl migration within a main group organometallic compound

D. Dakternieks*, A.E.K. Lim and K.F. Lim*,

Biol. and Chemical Sciences, Deakin University, Geelong, VIC 3217, AUSTRALIA

Competitive reactive pathways for dissociation of organotin cations.

Zero-point energy constraints in RRKM and non-RRKM molecules

Physical Chemistry Chemical Physics

D.A. McCormack and K.F. Lim*

Biol. and Chemical Sciences, Deakin University, Geelong, VIC 3217, AUSTRALIA

Constrained-classical mechanics is used to mimick quantized behaviour, i.e. preventing the flow of energy from vibrational zero-point motion to the reaction coordinate motion.

Probabilities for the $F+H_2 \rightarrow HF + H$ reaction by the Hyperquantization Algorithm: Alternative sequential diagonalization schemes

Phys. Chem. Chem. Phys.

V. Aquilanti, S. Cavalli, D. De Fazio, A. Volpi

Dipartimento di Chimica, Università di Perugia, 06123 Perugia, Italy

A. Aguilar, X. Giménez, and J. M. Lucas

Departament de Química Física, Universitat de Barcelona, 08028 Barcelona, Spain

This work reports on the performances of the Hyperquantization Algorithm in the symmetric hyperspherical coordinate representation for the $F + H_2$ reaction. The use of alternative sequential diagonalization schemes has greatly reduced the computing time and memory requirements. The effectiveness of the sequential diagonalization-truncation depends on the topology of the potential energy surface, which varies along different ranges of the hyperradius. The appearance at $\rho \sim 4a_0$ of the ridge line on the potential energy surface, which separates the reactant and product valleys, marks the transition between the regions of preferential applicability of two alternative ways to perform sequentially the diagonalization of the fixed- ρ Hamiltonian matrix.

Quantum Dynamics of Kinematic Invariants in Tetra- and Polyatomic Systems

R. G. Littlejohn and K. A. Mitchell

Department of Physics, University of California, Berkeley, California 94720 USA

V. Aquilanti

Dipartimento di Chimica dell'Università, 06100 Perugia, Italy

For the dynamical treatment of polyatomic molecules or clusters as n -body systems, the kinematic invariants are related to the three principal moments of inertia of the system. At a fixed value of the hyperradius (a measure of the total moment of inertia), the space of kinematic invariants is a certain spherical triangle, upon which angular coordinates can be imposed. It is shown that this triangle provides the 24-element (group O) octahedral tessellation of the sphere for $n = 4$ and the 48-element (group O_h) octahedral tessellation for $n \geq 5$. Eigenfunctions describing the kinematics of systems with vanishing internal and external angular momentum can be obtained in closed form in terms of Bessel functions of the hyperradius and surface spherical harmonics. They can be useful as orthonormal expansion

basis sets for the hyperspherical treatment of the n -body particle dynamics.

c. Conferences

1. THE 5th GORDON CONFERENCE ON GAS PHASE ION CHEMISTRY

Ventura, California, Feb. 28 - March 5, 1999

The program is now on the web at:

<http://www.unc.edu/depts/chemistry/gordon/index.html>

If this conference is of interest to you, please add this address to your bookmarks.

Tomas Baer, Conference Chair, Kenan Professor of Chemistry, Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290, Baer@unc.edu, <http://net.chem.unc.edu/faculty/tb/cftb01.html>

2. WORKSHOP ON "TIME-DEPENDENT QUANTUM MOLECULAR DYNAMICS"

Brian Head, Utah, March 13-17, 1999 The Henry Eyring Center for Theoretical Chemistry at the University of Utah and the Quantum Theory Project at the University of Florida wish to announce a workshop on "Time-Dependent Quantum Molecular Dynamics". At this time, there is space for 20 more attendees, in addition to the invited speakers and their selected graduate students/postdocs. More information on the workshop and a registration form may be found at the web site:

<http://www.hec.utah.edu/brianhead/>.

Please download the registration form and mail it to me at the address below if you are interested in attending.

This workshop should prove to be a very stimulating meeting focused on a topic which has emerged as one of the central themes in theoretical chemistry.

3. American Chemical Society

Anaheim, California, March 21-25, 1999

The following list gives the symposia that are planned for the Anaheim, California meeting of the American Chemical Society (March 21-25, 1999). Abstracts are due November 1, 1998. If you have a contribution that belongs to one of the symposium topics, please send it to one of the organizers of the symposium. Abstracts on other topics should be sent to me. These will be included in a general poster session. Further information concerning this meeting and about other activities of the physical division can be seen at

<http://hackberry.chem.niu.edu/PHYS>

Four copies of 150-word abstract (original on ACS Abstract Form) to symposium organizer by November 1, 1998. Forms are available from <http://www.acs.org>

Linear Polyene Spectroscopy: A Celebration of the Scientific Career of Bryan Earl Kohler, B. S. Hudson, Dept. of Chemistry, Syracuse Univ., Syracuse, NY 13244-4100, (315) 443-5805, fax (315) 443-4070, email: bshudson@syr.edu

Unimolecular Reactions and Intramolecular Dynamics, S. J. Klippenstein, Dept. of Chemistry, Case Western Reserve University, Cleveland, OH 44106; 216-368-6916, fax (216) 368-3006, email: sjk5@po.cwru.edu, David Perry, Department of Chemistry, University of Akron, Akron, OH 44325, (216) 972-6825, fax (216) 972-6990, email: DPerry@uakron.edu

Heavy Element Complexes: The Convergence of Theory and Experiment, (Joint with NUCL), James V. Beitz, Chemistry Division, Argonne National Laboratory, Argonne IL 60439, (630)252-7393 email: beitz@anlchm.chm.anl.gov; David L. Clark, G. T. Seaborg Institute, Mail Stop E500, Los Alamos National Laboratory, Los Alamos, NM 87545, email: dlclark@lanl.gov

Radicals in Condensed Phases, David Bartels, Chemistry Division, Argonne National Laboratory, Argonne IL 60439, (630)252-3485 fax: (630) 252-4993 email: bartels@anlchm.chm.anl.gov; Greg Schenter, Environmental Molecular Science Lab, MS K1-96, Pacific Northwest National Laboratory, Batelle Blvd, Richland, WA 99352, (509) 375-2945, email: gk_schenter@pnl.gov

Physical Chemistry of Sol-gel Materials, Jeff Zink, Department of Chemistry and Biochemistry, University of California, 405 Hilgard Ave., Los Angeles, CA 90095-1569, 310-825-1001, fax 310-206-9880,

zink@chem.ucla.edu; Bruce Dunn, Department of Materials Science and Engineering, UCLA, Los Angeles CA 90095, 310-825-1519, email: dunn@seas.ucla.edu

Dynamics/Structure at Electrochemical Interfaces by New Spectroscopic Probes and Approaches, Andrzej Wieckowski, Chemistry Department, University of Illinois, Urbana, IL 61801, (217)333-7943, fax: (217)333-0711 email: andrzej@aries.scs.uiuc.edu; Joseph T. Hupp, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, (847)491-3504, fax (847)491-7713, email: jthupp@chem.nwu.edu
Liquids and Interfaces (in honor of Doug Henderson), Randall Shirts Department of Chemistry, Brigham Young University, Provo UT 84602-5700, 801-378-4290, fax: 801-378-5474, email: rbshirts@chemdept.byu.edu

Frontiers of Statistical Mechanics (in honor of Ben Widom), A.D.J. Haymet, Department of Chemistry and Institute for Molecular Design, University of Houston, 4800 Calhoun, Houston, TX 77204-5641, 713-743-2781, fax: 713-743-2709 email: haymet@uh.edu

4. Electronic and structural dynamics of light-induced processes in bacteriorhodopsin

University of Lausanne (Switzerland), 9-10 April 1999

Chairmen: M. Chergui and S. Haacke

<http://www.unil.ch/ipe>

Recent progress in protein synthesis and spectroscopy is a strong motivation for a workshop focusing on bacteriorhodopsin and its mutants. The central subject of the workshop is the relation between structure and photosensitive functions of the BR protein, with special emphasis on the dynamics, both from the experimental and theoretical point of view. Addressing a specific community and a well-defined topic, the workshop will allow for a very informal and direct exchange of information and ideas.

Topics to be covered include BR synthesis and mutagenesis, X-ray diffraction, steady-state and ultrafast spectroscopy, as well as theoretical modelling.

The following invited speakers have so far confirmed their participation:

P. Anfinrud (Bethesda, USA), G.H. Atkinson (Tucson, USA), E. Bamberg (Frankfurt), Ch. Bressler (UNI Lausanne), G. Bldt (Jlich), M. Chergui (UNI Lausanne), L.O. Essen (MPI, Munich), J. Heberle (Jlich), R. Henderson (MRC, Cambridge), E. Landau (Biozentrum Basel), R. Neutze (Uppsala, Sweden), M. Ottolenghi (Jerusalem), E. Pebay - Proula (IBS, Grenoble), M. Sheves (Rehovot, Israel), K. Schulten (Urbana, USA), V. Sundstroem (Lund, Sweden), W. Zinth (LMU, Munich).

The workshop will take place at the campus of the University of Lausanne, a green park area next to Lake Geneva, offering an impressive view of the Alps. Accommodation will be downtown (see below for hotel reservations) and can be reached easily within 20 min by public transportation. Lausanne is directly linked through frequent train connections with the airports in Geneva (40 min) and Zurich (2h 45min), and is also easily accessible by train from other major European cities.

Participants are encouraged to submit contributions in the form of posters. These will be posted close to the conference room and will be accessible throughout the workshop. A one-page abstract should be submitted before March, 30th 1999. All contributions are accepted without selection.

Accommodation and travel information: The approximate prices for hotels in Lausanne range from Sfr 110.- to 150.- /night for a single room. Please consult the workshop web site <http://www.unil.ch/ipe> for more information and hotel registration forms. We recommend you to book your hotel via us, as the University benefits from special rates.

The registration fee will be including attendance at the workshop, workshop dinner, and coffee breaks.

Registration and deadlines: the registration form should be copied to your e-mail answer and sent before March 15th, 1999 to QD@ipmc.ipe.unil.ch or sandrine.massonet@ipmc.ipe.unil.ch

Further information about the workshop can be obtained from the Web site: <http://www.unil.ch/ipe>

5. Rovibrational Bound States in Polyatomic Molecules

Aberdeen, UK, 11-14 April 1999

This specialist workshop is sponsored by CCP6 (the UK Collaborative Computational Project on Heavy Particle Dynamics). The meeting will focus on the challenging problems associated with wide amplitude rovibrational bound state calculations in tetraatomic molecules and larger. Topics covered will include:

coordinate systems; derivation of exact kinetic energy operators; representation of potential energy surfaces; choice of basis functions; strategies such as the discrete variable representation and contraction schemes; large matrix diagonalisation methodologies; and opportunities offered by supercomputer architectures.

We intend to limit participation to about 30 keenly interested people, with 12 invited talks. The format will be "Gordon Conference style", with sessions in the morning and evening but afternoons free.

Invited speakers will include:

Zlatko Bacic (USA), Tucker Carrington (Canada), David Clary (UK), Benny Gerber (Israel), Nicholas Handy (UK), Lauri Halonen (Finland), Claude Leforestier (France), Kevin Lehmann (USA), David Nesbitt (USA), Jonathan Tennyson (UK), Ad Van der Avoird (Netherlands)

Organising committee: Mark Law, e-mail: M.M.LAW@ABDN.AC.UK, Jeremy Hutson, Ian Atkinson,

For further information please consult the conference Web page

<http://www.abdn.ac.uk/~che194/research/rovib99/>

6. One day meeting on Energetic Molecule and Cluster Interactions with Solid Surfaces

The Ion and Plasm surface Interactions Group of the Institute of Physics have organised a 1 day meeting on 15/4/99 in conjunction with the IOP congress in Manchester entitled "Energetic Molecule and Cluster Interactions with Solid Surfaces".

Please see the web page on <http://www.IOP.org/IOP/Confs/EMCISS/> or reply to this email for further details. Late abstracts will still be accepted. Cost for students is cheap at only £ 10.

Roger Smith, School of Mathematics and Physics, Loughborough University, Loughborough LE11 3TU, UK. tel: 44 1509 223192 fax: 44 1509 223969 Web :

<http://info.lboro.ac.uk/departments/ma/staff/rogerSmith.html>

7. An International Conference in Electronic Format sponsored by Gordon and Breach

Conference Chair: Professor Nick Quirke, Imperial College, Editor-in-Chief, Molecular Simulation Journal

Dates: 19 April - 4 May '99

URL: <http://molsim.vei.co.uk/>

** Now calling for PAPERS - Submit your abstract via the on-line form at

<http://molsim.vei.co.uk/submissions/index.html> N.B. Deadline for abstracts = 1 March 1999

** FREE Registration to attend the conference now available - Fill in the form at

<http://molsim.vei.co.uk/register/index.html>

DESCRIPTION

The international journal Molecular Simulation is sponsoring a virtual conference on the latest applications and techniques in the field. The conference will bring together experts, in a wide range of disciplines encompassed within the physical and biological sciences, using molecular simulation and related techniques.

An important aim of the meeting is to foster cross fertilisation of ideas, algorithms and applications between them. Sessions will include papers on topics in physics, chemistry, materials science, biology and pharmacology. Comment and discussion will be encouraged and the resulting material will be edited and form part of the proceedings.

The format of the virtual conference will be formal sessions with invited and contributed papers, posters and subsequent interactive discussions with authors, where comment and criticism will be sought on the formal lectures (along the lines of a Faraday Discussion). During the conference all material will be accessible at the conference Web site and accepted papers will be published after the end of the conference (following refereeing and editing) in Molecular Simulation.

TOPICS, CHAIRS and SPEAKERS

The six sections will cover the following topics. Also find listed the chairs for each topic and some of the invited speakers confirmed so far.

Applications:

1. Frontiers of Materials Science Chairs: Prof. Alain Fuchs, Prof. C R A Catlow Invited Speakers:

2. Novel Applications in Chemistry and Physics Chairs: Prof Donald Brenner, Dr. Deepak Srivastava Invited Speakers:

3. Computer based Modelling, Simulation, and Analysis of Biological and Pharmacological Systems Chairs: Prof. Graham Richards, Dr. Jeffrey L. Nauss Invited Speakers: Steve Doughty, Vijay Gombar, Ian Haworth, Prof. Mati Karelson, Dave Winkler

Methodology:

4. Advances in Mesoscale Simulation Methodology Chairs: Dr. Julia Yeomans, Dr. Dave Nicolaides Invited Speakers: Bruce Boghosian, Hudong Chen, J.G.E.M. Fraaije, Anatoly Malevanets

5. Non Equilibrium and Monte Carlo Simulation Chairs: J.M.D.MacElroy, B.E.Ph.D., Grant S. Heffelfinger, Ph.D. Invited Speakers: Prof. David M. Ford, Prof. Akira Miyamoto, Dr. David Nicholson, Prof. Tomoshige Nitta, Dr. Aidan Thompson, Dr. Karl P. Travis,

6. Advances in Quantum Simulation Chairs: Dr. Dominic King-Smith, Dr. M.C. Payne Invited Speakers: Mike Gillan, Pablo Ordejon, Dr. Mike Payne, Gustavo Scuseria, Alain St-Amant

8. International Symposium on The Treatment of Complex Chemical Systems: New Concepts in Theory and Experiment in honor of Professor Jürgen Brickmann on the occasion of his 60th birthday

Department of Chemistry, Darmstadt University of Technology, May 27 - 29, 1999

Scope of the Symposium: Large and complex systems provide some of the most challenging experimental and theoretical problems in modern chemistry. By complex systems, it is meant that the systems as well as the models used should reflect chemical conditions in a realistic way. This requires the proper and simultaneous treatment of different species and phases. The purpose of this symposium is to survey recent research in the development of new model scenarios, new theoretical approaches and simulation techniques of complex systems and processes as well as subtle experimental techniques in order to study these kinds of systems.

It is the aim of this meeting to discuss various ways to overcome the limitations of individual methods by combining different approaches and to demonstrate in this way the power of new concepts and technologies. The invited speakers are selected from a wide variety of fields ranging from philosophy to preparative chemistry. Therefore, the meeting is expected to be of interest to both experimentalists and theorists from all branches of science, as well as mathematicians and computer scientists.

D. Avnir, Jerusalem (Israel); V. Aquilanti, Perugia (Italy); H. Baumga"rtel, Berlin (Germany); R.S. Berry, Chicago (USA); P. Bopp, Bordeaux (France); E. Braendas, Uppsala (Sweden); L. Cederbaum, Heidelberg (Germany); B. Gerber, Jerusalem (Israel); E. Gudowska-Nowak, Krakow (Poland); R. Kniep, Darmstadt (Germany); G. Kothe, Freiburg (Germany); H. Kubinyi, Ludwigshafen (Germany); R. D. Levine, Jerusalem (Israel); H. Limbach, Berlin (Germany); P. Mezey, Saskatchewan (Canada); J. Mittelstrass, Konstanz (Germany); K. Schulten, Urbana-Champaign (USA); A. Sgamellotti, Perugia (Italy); A. Skerra, Darmstadt (Germany); J. Weber, Geneva (Switzerland); E. Yurtsever, Istanbul (Turkey);

Registration fee: none. Hotel rooms can be reserved by contacting the tourcongress bureau Darmstadt, Luisenplatz 5, D-64283 Darmstadt, phone: (+49) 6151-13 20 7, fax: (+49) 6151-13 20 75 Please register on-line at: <http://www.pc.chemie.tu-darmstadt.de/symposium1999/>

Please send correspondence to: Dr. Hans-Jürgen Bär, Institute of Physical Chemistry, Darmstadt University of Technology, Petersenstr. 20, D-64289 Darmstadt, Germany, Fax: (+49) 6151/164298, Email: hjb@pc.chemie.tu-darmstadt.de

9. 18th International Symposium on Molecular Beams 1999

Ameland, The Netherlands, May 30 - June 4, 1999

Chairmen: Steven Stolte (VU Amsterdam) and Gerard Meijer (KU Nijmegen)

A Web-page is being prepared and will be announced in the next issue of MDN and on the department home-page: <http://www-mlf.sci.kun.nl/mlf/>

10. 54th OHIO STATE UNIVERSITY INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY June 14-18, 1999, Columbus, Ohio, USA

EXECUTIVE COMMITTEE Terry A. Miller, Chair, Frank C. DeLucia, Eric Herbst, C. Weldon Mathews, Russell M. Pitzer

INTERNATIONAL ADVISORY COMMITTEE Phil Bunker (NRCC), Chair* Michael A. Duncan (U. Georgia) Wolfgang Ernst (Penn. State U.)* Michael C. L. Gerry (U. British Columbia) Yen-Chu Hsu

(Academia Sinica) Jaan Laane (Texas A&M U.) Ronald M. Lees (U. New Brunswick)* John P. Maier (U. Basel) A. Robert McKellar (NRC) W. Leo Meerts (U. Nijmegen) Klaus Muller-Dethlefs (York U.) David Nesbitt (U. Colorado) Stewart Novick (Wesleyan U.)* Agnes Perrin (University Paris Sud) Eric Rohlfing (Sandia National Labs) David Dale Skatrud (ARO) Richard D. Suenram (NIST) Keiichi Tanaka (Inst. Molecular Science) * steering committee member

For additional information contact: Terry A. Miller, Chair International Symposium on Molecular Spectroscopy Department of Chemistry 120 West 18th Avenue Columbus, Ohio 43210 USA 614-292-2569 (phone), -1948 (FAX) e-mail: mss@molspect.mps.ohio-state.edu

<http://molspect.mps.ohio-state.edu/symposium/>

INFORMATION FOR 54th MEETING

PLENARY SPEAKERS

Geoff Blake, California Institute of Technology Shuji Saito, Institute for Molecular Sciences Paul Davies, Cambridge University Richard Saykally, University of California, Berkeley Takeshi Oka, University of Chicago, Lippencott Award Winner Peter Toennies, University of Gottingen Brooks Pate, University of Virginia, Coblentz Award Winner

SPECIAL SESSIONS Several special mini-symposia are planned for this year's meeting. Bill Kirchhoff, Department of Energy, is organizing a session entitled, "Spectroscopy Related to Combustion" which will cover the spectroscopy of molecules relevant to combustion processes, the application of spectroscopy to the characterization of chemical dynamics, as well as spectroscopic means to monitor the processes themselves.

Invited speakers will include Phil Paul, Sandia National Labs, Marsha Lester, University of Pennsylvania, and Ronald Hanson, Stanford University. A second mini-symposium is being organized by Eric Herbst, Ohio State University, on the subject of "Spectroscopy of the Heavens" covering molecules observed or

observable as well as new spectroscopic approaches to astronomical observations. Invited speakers for this mini-symposium include Louis Allamandola, NASA/AMES, and Gisbert Winnewisser, Universitat zu Koeln. A third mini-symposium is being co-organized by Rick Suenram, NIST, and David Skatrud, Army Research Office on "Spectroscopy and Environmental Monitoring." The symposium will encompass the use of molecular spectroscopy for a variety of applications including atmospheric sensing, environmental and treaty compliance monitoring, industrial process control and optimization, etc. Invited speakers will include Phil DeCola, NASA, and Kevin McNesby, ARL, and J. D. Tate, Dow Chemical. A session on theory is being organized by Russell Pitzer, Ohio State University, featuring a talk by Jeppe Olsen, Lund University.

ELECTRONIC ACCESS We continue to emphasize electronic communication with respect to the Symposium. These efforts are driven by our dual desire to provide the best service while minimizing costs. The key place to learn symposium details is our WWW site, <http://molspect.mps.ohio-state.edu/symposium/>. All the information in the flyer plus much more is available there. When the preliminary program (containing complete abstracts for those submitted electronically) is completed in early April, it will be immediately available at the WWW site, and you will be informed of its availability by email (for all on our email list). We strongly encourage abstracts to be submitted electronically. Detailed instructions for electronic abstract submission (EAS) can be obtained by email or by viewing our WWW site. Please note that we will maintain a test service so you can preview your abstract on our machine before you make a final submission. Please visit our WWW site to learn about the services, e.g., template, examples, help pages, etc, that we are providing to make electronic abstract submission as simple as possible. We plan again to produce the entire abstract book electronically.

PRE-REGISTRATION In an effort to make it easier to pre-register, especially for those with currency exchange problems, we have again worked out an arrangement with the Ohio State dorms. This year you will be able to charge your entire pre-registration (conference and dorm) fee to your Visa or MasterCard credit card (see registration information). For those few not pre-registering, you will be able to charge your dorm accommodations on site, but NOT your Symposium registration fee. We would encourage those for whom it does not represent a major inconvenience to continue to pay by check, as you realize that credit card use comes at a price to the Symposium.

11. XVI INTERNATIONAL CONFERENCE ON MOLECULAR ENERGY TRANSFER (COMET XVI)

"La Cittadella", Assisi, ITALY, June 20-25, 1999

<http://www.chm.unipg.it/chimgen/mb/cong/comet.html> e-mail: comet@dyn.unipg.it

The XVI International Conference On Molecular Energy Transfer, COMET XVI, will be held at "La Cittadella", a conference facility in Assisi, ITALY, 20-25 June 1999. Assisi is a unique medieval town rich in art masterpieces. It is located in a beautiful landscape, 25 km east of Perugia, the capital of the Umbria region known as the "green heart" of Italy. The COMET is a Gordon type conference held every two years alternating between the USA and Europe.

The purpose of the 1999 conference is to survey recent advances, undertake stimulating discussions, generate new ideas, and map out future directions in the field of molecular energy transfer. The scientific program will concentrate on dynamical aspects of molecular energy transfer. Particular emphasis will be given to State-to-state dynamics Inelastic and reactive collisions Unimolecular reactions Ion reaction dynamics State-selected (inter- and intra-molecular) energy transfer Internal vibrational redistribution Energy transfer in condensed phase Clusters and hydrogen bonded systems Photodissociation Imaging techniques Non-adiabatic processes Open-shell dynamics and spectroscopy Transition state spectroscopy Femtosecond dynamics

INVITED SPEAKERS

M.H. Alexander (University of Maryland), M.N.R. Ashfold (University of Bristol), G. Balint-Kurti (University of Bristol), J.M. Bowman (Emory University), D.C. Clary (University College London), F.F. Crim (University of Wisconsin), O. Dutuit (Universit de Paris-Sud, Orsay), G.R. Fleming (University of California, Berkeley), G.W. Flynn (Columbia University), D.R. Herschbach (Harvard University), F. Huisken (Max-Planck-Institut, Goettingen), M.I. Lester (University of Pennsylvania), J.C. Light (University of Chicago), W.C. Lineberger (JILA, University of Colorado), K. Liu (IAMS, Academia Sinica, Taipei), H.H.J. ter Meulen (University of Nijmegen), W.H. Miller (University of California, Berkeley), E. Murad (Air Force Research Lab, Hanscom AFB), R. Naaman (Weizmann Institute, Rehovot), D. Nesbitt (JILA, University of Colorado), D.M. Neumark (University of California, Berkeley), G.A. Parker (University of Oklahoma), H. Reissler (University of Southern California), G. Scoles (Princeton University), J.P. Simons (Oxford University), T. Suzuki (IMS, Okazaki), F. Vecchiocattivi (University of Perugia), R.N. Zare (Stanford University),

Piergiorgio Casavecchia (Co-Chair), Dipartimento di Chimica, Universit di Perugia, 06123 Perugia, Italy, Phone: (+39) (075) 585-5514, Fax: (+39) (075) 585-5606, Email: piero@dyn.unipg.it

Antonio Lagana' (Co-Chair), Dipartimento di Chimica, Universit di Perugia, 06123 Perugia, Italy, Phone: (+39) (075) 585-5515, Fax: (+39) (075) 585-5606, Email: lag@dun.unipg.it

The local organizing committee includes the members of the Perugia Group: V. Aquilanti, N. Balucani, B. Brunetti, R. Candori, D. Cappelletti, S. Cavalli, S. Crocchianti, S. Falcinelli, G. Grossi, G. Liuti, E. Luzzatti, F. Pirani, F. Vecchiocattivi, G.G. Volpi.

Note that COMET XVI will be followed immediately after by the "Workshop on Quantum Reactive Scattering" (Perugia, Italy, 25-27 June 1999) and by the 1st European Computational Chemistry School on "Molecular and Reaction Dynamics" (Perugia, Italy, June 28-July 4, 1999).

Information will be continuously updated on the Web site. On January 1999 it will be e-mailed to people on the Conference mailing list. To be added to the mailing list, please fill out the form and mail or fax it. You can also pre-register at our Web Site: <http://www.chm.unipg.it/chimgen/mb/cong/comet.html>

The Second Announcement will include more specific details about the call for papers, registration, fees, traveling and housing.

PRE-REGISTRATION FORM

To receive further information, register at our WWW site

<http://www.chm.unipg.it/chimgen/mb/cong/comet.html> .

COMET XVI, Prof. P.Casavecchia, Dipartimento di Chimica, Universita' di Perugia, Via Elce di Sotto, 8, 06123 PERUGIA, ITALY, FAX: (39) 075 5855606, e-mail comet@dyn.unipg.it

12. WORKSHOP ON QUANTUM REACTIVE SCATTERING

Perugia, Italy, 25-27 June, 1999

The meeting, which will be sponsored by the D9 COST Action in Chemistry, will hopefully be attended by most of the world experts in the field, and will be run in the same spirit and with the same objectives as the four previous workshops on reactive scattering (Cambridge UK, 1990, organised by David Clary, Cambridge USA, 1994, organised by Yan Sun and Michael Baer, Nottingham UK, 1995, organised by David Clary and David Manolopoulos, and Telluride, Colorado, 1997, organised by Joel Bowman).

The emphasis of the workshop will be on the latest theoretical developments and the most impressive recent calculations. The most ingenious new approximations in reactive scattering will also be discussed.

Interesting new directions for the application of reactive scattering theories will also be discussed, with special attention towards systems of increasing complexity, according to the aims of the D9 COST Action. For information, contact V. Aquilanti [aquila@dyn.unipg.it] or A. Laganà [lag@dyn.unipg.it]

13. EUROPEAN COMPUTATIONAL CHEMISTRY SCHOOL: MOLECULAR AND REACTION DYNAMICS

Perugia, Italy, June 28 - July 4, 1999

The European Computational Chemistry Groups have started a European School on "Molecular and Reaction Dynamics" to be held in Perugia (Italy) every fourth year starting from its first edition (June 28 - July 4, 1999). The School will be jointly run by the Department of Chemistry and the Computer Center of the University of Perugia.

Morning sessions will be devoted to chemical theory and problems while the afternoon sessions will be devoted to Computer Science advances and Computational Chemistry applications (two plenary lectures dealing with fundamental aspects of reactivity and dynamics calculations of molecular systems during the morning session; one lecture on computing advances and a three hour long tutorial devoted to Molecular and Reaction Dynamics computational applications in the afternoon).

Have already accepted to deliver lectures G.C. Schatz, M. Vanneschi, G.A. Parker, A. Kupperman, G.G. Balint Kurti, J. Zhang, D. Kouri, G.D. Billing, M. Robb, F. Bernardi.

For further information contact Prof. Antonio Lagana'

Dipartimento di Chimica, Università di Perugia, Perugia (Italy),

email lag@unipg.it,

tel. +39.75.5855515, tel. +39.75.5855606.

Information will also appear soon in the web (www.chm.unipg.it/chimgen/mb/theo1/gicc.html)

14. THE 1999 AMERICAN CONFERENCE ON THEORETICAL CHEMISTRY (ACTC)

Boulder, June 27-July 2 1999

Information: Prof. Eric Heller

heller@physics.harvard.edu

15. STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS

Bretton Hall, University of Leeds, 5-7 July 1999

Faraday Discussion No 113 will be held at Bretton Hall, University of Leeds, 5-7 July 1999 on the theme of "Stereochemistry and Control in Molecular Reaction Dynamics". The Discussion will focus on comparing frequency, temporal and phase control strategies to probe elementary chemical processes. Further details are available at

<http://www.chem.leeds.ac.uk/faraday113/>

Experimental and theoretical papers will be particularly welcome in the following areas:

- * High resolution studies (both frequency and time resolved) of molecular photodissociation of photoinitiated processes

- * Control of reactivity via collision energy, selective vibration of reagents, or reagent alignment

- * Demonstrations of active or coherent control of chemical processes

At this time we are seeking Titles and Abstracts of about 300 words. The DEADLINE for submission of these proposed contributions is FRIDAY 29 MAY 1998. They should be sent to Dr. BJ Whitaker, School of Chemistry, University of Leeds, LS2 9JT and may be in any form - manuscript, fax, whatever but electronic attachments will be particularly cherished. Papers should be concerned with new, unpublished work. The full proceedings of the Discussion will be published late in 1999, but papers accepted for discussion will be

circulated to all participants before the meeting in July 1999. Those unfamiliar with the unique format of Faraday Discussions can obtain more information from the URL above.

Benjamin J Whitaker, School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK
email: benw@chem.leeds.ac.uk, tel: (44) 113 233 6580, fax: (44) 113 233 6565

16. 1999 EGAS Conference : 6th - 9th July 1999 in Marseille

European Group for Atomic Spectroscopy (EGAS) is a group within the Atomic and Molecular Physics Division of the European Physical Society.

EGAS organises an annual conference on topics in the spectroscopy of atoms and small molecules, but also including a strong emphasis on the related fields of light-atom interactions, laser cooling and trapping, atom optics and B.E.C. The conference aims to bring together leading participants in these fields, but to remain most accessible to young researchers, especially graduate students. To this end plenary speakers are asked to include a tutorial element in their talks and great efforts are made to keep the costs of the meeting as low as possible. There is no formal membership requirement for EGAS: the membership simply comprises the people who attend the conference. All are welcome.

The 1999 EGAS Conference will be held in Marseille from the 6th - 9th July. Full details can be found on the Conference Web Site, where you can also pre-register in order to receive further details.

The address is:- <http://www.up.univ-mrs.fr/~wegas99/>

Alternatively the organisers can be contacted by e-mail at:-

egas99@newsup.univ-mrs.fr

A permanent web site for EGAS is maintained by the University of Liege at

<http://www.ulg.ac.be/ipne/data/egas/egas.html>, where general details of the Group can be found.

17. THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE

Split Rock Resort in Lake Harmony, Pennsylvania, USA, July 18-23, 1999

James J. Valentini, Chair Department of Chemistry Columbia University New York, NY 10027 USA

James T. Muckerman, Vice-Chair Department of Chemistry Brookhaven National Laboratory Upton, NY 11973 USA

Description of the Conference

The Dynamics of Molecular Collisions Conference focuses on all aspects of molecular collisions—experimental and theoretical studies of elastic, inelastic, and reactive encounters involving atoms, molecules, ions, clusters, and surfaces—as well as half collisions—photodissociation, photo-induced reaction, and photodesorption. The Conference began as a Gordon Conference in 1965, and though it now operates independently, retains the Gordon Conference format and spirit.

Meeting Site

The meeting will be held at The Resort at Split Rock in eastern Pennsylvania, a five-hundred-acre year-round resort situated on Lake Harmony and surrounded by the forests, lakes and streams of the Pocono Mountains. The Resort is located 1-1/2 to 2 hours from New York City airports, while the Wilkes-Barre International and Lehigh Valley International Airports are only 30 and 50 minutes away.

Split Rock has abundant recreational facilities, including 18 holes of championship golf, an 18 hole miniature golf course, 2 indoor pools, 1 outdoor pool, a swimming lagoon, 9 indoor and outdoor tennis courts, racquetball, archery, bocci ball, shuffleboard, softball, volleyball, health club and fitness center, billiards room, bowling alley with 8 lanes, first run movie theater, fishing, boat rides, paddle boats, water skiing, outdoor barbecues, hiking, and biking.

More information on Split Rock is available at the Resort web site, <http://www.splitrockresort.com>.

Meeting Program

The XVIIth Conference will have morning sessions on Monday through Friday, and evening sessions Monday through Thursday. In each session the first talk will be an overview of the topic of that session. Afternoons are free for discussions and recreation. Session topics and speakers are:

Bimolecular Reaction Dynamics—Experiment Paul Dagdigian (Johns Hopkins University) Richard Zare (Stanford University) Arthur Suits (University of California, Berkeley) Hansjuergen Loesch (University of Bielefeld)

Bimolecular Reaction Dynamics–Theory Russell Pack (Los Alamos National Laboratory) John Zhang (New York University) Stephen Gray (Argonne National Laboratory) Antonio Varandas (University of Coimbra) Collisions at Surfaces Barbara Garrison (Pennsylvania State University) J. Michael White (University of Texas) Hua Guo (University of New Mexico)

Collisions at Ultralow Temperatures Daniel Heinzen (University of Texas) Paul Julienne (NIST, Gaithersburg) William Stwalley (University of Connecticut)

Control of Molecular Dynamics David Tannor (Weizmann Institute) Robert Gordon (University of Illinois, Chicago) Stephen Leone (University of Colorado) Gustav Gerber (University of Wurzburg)

Dynamics in Clusters James Lisy (University of Illinois) Michael Heaven (Emory University) Zlatko Bacic (New York University) Koichi Yamashita (University of Tokyo)

Eigenstate Resolved Dynamics Thomas Rizzo (EPH, Lausanne) Patrick Vaccaro (Yale University) Amit Sinha (University of California, San Diego)

Photodissociation Dynamics Reinhard Schinke (Max-Planck-Institut) Gabriel Balint-Kurti (University of Bristol) Gregory Hall (Brookhaven National Laboratory)

Nonadiabatic Processes Robert Parson (University of Colorado) Sharon Hammes-Schiffer (University of Notre Dame) Laurie Butler (University of Chicago)

Posters

Split Rock has extensive and very attractive facilities for presentation of posters. Instructions on how to submit posters will be given in the Third Circular, to be distributed March 1.

Registration and Fees

Registration and payment of fees will be done through the Resort office. Instructions on how to register will be given on March 1 in the Third Circular.

Fees for room and board will be: Double occupancy: 602; *singleoccupancy* :848

Registration fee: \$50 (waived for graduate students and postdocs)

It is anticipated that there will be some monies available for graduate student scholarships.

Conference Web Site and Email

A conference web site will be active beginning March 1. Details will be provided in the Third Circular to be released on that date.

Email regarding the Conference should be sent to the Chair at jjv1@chem.columbia.edu.

18. ICPEAC XXI

July 22 - 27, 1999, Sendai, Japan

The twenty first meeting of the International Conference on the Physics of Electronic and Atomic Collisions will be held July 22 - 27, 1999 (Thursday - Tuesday) in Sendai, Japan. Sendai is the economic and cultural center of the Tohoku (north- eastern) region of Japan. It is located near the ocean 200 miles north of Tokyo. Further information may be obtained from Prof. Michio Matsuzawa, Applied Physics & Chemistry, University of Electro-Communications, Tokyo, 182-8585, Japan. Fax: 81-424-43-5505 e-mail michio@pc.uec.ac.jp Homepage: <http://power1.pc.uec.ac.jp/Sendai>

19. PHOTO-DYNAMICS AND REACTION DYNAMICS OF MOLECULES

Inst. for Molec. Science, Okazaki, Japan, July 31(Sat) - August 2(Mon), 1999.

Organizers: Hiroki Nakamura and Koichiro Mitsuke, Inst. Molec. Sci., Okazaki. e-mails: nakamura@ims.ac.jp, mitsuke@ims.ac.jp, Home page: <http://www.ims.ac.jp/pdrdm/>

Scope of the symposium

This satellite meeting of The XXI ICPEAC in Sendai is primarily intended to exchange scientific information and discussions among scientists who are interested in the studies of dynamics of molecules such as molecular photo-ionization, molecular photo-excitation and dissociation, molecular reaction dynamics, and transition-state spectroscopy. The scientific program will be composed of invited talks, some oral presentations and poster sessions, covering both experimental and theoretical aspects.

The invited talks are expected to cover the following broad areas: Inner shell photoionization and subsequent decay dynamics, Multiple ionization and dichroism, Dynamics of superexcited molecules, Excited atom ionization and time-resolved spectroscopy, Photoionization complete experiments, Ionization of oriented

molecules, laser investigation of molecular photodissociation, Multiphoton experiments, VUV laser experiments, Reaction dynamics involving excited-state atoms, Dynamical behaviors of molecules in an intense laser field, Reaction of highly-charged ions, Transition-state spectroscopy, Theory of chemical reaction dynamics

20. Gordon Research Conference on: Dynamics at Surfaces

Proctor Academy, Andover, New Hampshire, USA, August 8-13, 1999

Chair: Aart Kleyn FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands Email: KLEYN@AMOLF.NL

Vice-Chair: Bruce Kay Pacific NW Natl Lab, Environm Mol Sci Lab, Richland, WA

The next meeting in this very dynamic series will be held again at Proctor Academy. The meeting will be in the same spirit as the very successful preceding ones, both in the sessions and other entertainment.

Topics of this Gordon Research Conference will include: Adsorption-Desorption, Adsorbate Vibrations, Atmospheric Surface Science, Charge Transfer, Diffusion and Growth, Gas-Surface Scattering, Liquid Surfaces, Nano-Scale Studies and Manipulation, Nano-Tribology, Photo-Dynamics and Chemistry, Surface Reactions and Catalysis, Best Student / Postdoc Poster Talks.

Information concerning the conference can be found at: <http://www.grc.uri.edu/programs/1999/surfaces.htm>

21. Microsymposium on Principles of molecular chirality and its significance for all branches of chemistry Berlin, 15 and 16 August 1999(during IUPAC congress)

Program available by January, deadline for oral contributions 31 December 98) Chairman Prof. Martin Quack, Lab. for Physical Chemistry, ETH Zuerich (Zentrum), CH 8092 Zuerich, Switzerland, Fax 01-6321021

22. 25th International Symposium on Free Radicals

Flagstaff, Arizona, August 15-20, 1999.

**To receive future notices, pre-register at our WWW site. <http://frs.mps.ohio-state.edu/frs>

Organizing Committee: R. F. Curl (Houston); M. Heaven (Atlanta); T. A. Miller (Columbus), Chair; T. Steimle (Tempe), Treasurer;

Additional information: email: frs@frs.mps.ohio-state.edu, <http://frs.mps.ohio-state.edu/frs>, or contact Terry A. Miller, 25th International Free Radicals Symposium, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus Ohio USA 43210

SCIENTIFIC PROGRAM

A wide variety of topics will be covered by papers and discussions: Spectroscopy of radicals, Dynamics and reaction kinetics, theory and experiment, Structure of free radicals, Molecular ions and molecules in excited states, Free radicals and atmospheric chemistry, Interstellar spectroscopy and chemistry, Free radicals as reaction intermediates, Free radicals in applied research, Production and observation techniques

There will be invited talks covering the above topics given by the following persons who have agreed to participate: A. Carrington (Southampton), P. Casavecchia (Perugia), P. Chen (Zurich), D. Clary (London), F. Crim (Madison), J. Doyle (Cambridge, Mass.), B. Ellison (Boulder), Y. Endo (Tokyo), K. Evenson (Boulder), Y. P. Lee (Hsinchu), J. Maier (Basel), M. McCarthy (Cambridge, Mass.), T. Oka (Chicago), F. S. Rowland (Irvine), T. Sears (Upton, NY), F. Temps (Kiel), V. Vaida (Boulder), G. Winnewisser (Cologne), A. Wodtke (Santa Barbara)

23. IAU Symposium 197 'Astrochemistry: from molecular clouds to planetary systems' Sogwipo, South Korea, August 23 - 27, 1999

This symposium is organized by the IAU working group on Astrochemistry (D.A. Williams (chair); E.F. van Dishoeck (secretary)) and will cover various topics in molecular astrophysics, including Basic molecular processes: gas-phase and gas-grain interactions; Physics and chemistry of star-forming regions: shocks, jets, PDR's and masers; Molecules in circumstellar disks; Solar system connection: comets, meteorites and IDPs; Chemistry in the inner and outer solar nebula; Atmospheres of planets and brown dwarfs; Diffuse and translucent clouds; Molecules and dust formation in circumstellar envelopes around late-type stars.

For further information, see <http://www.issa.re.kr/~iau197/>. To receive future mailings, send e-mail to: iau197@hanul.issa.re.kr

24. CCP5 ANNUAL MEETING 1999

SIMULATION OF CLUSTERS AND INTERFACES at the School of Chemistry, University of Birmingham, UK, 6-8th September 1999

The UK's EPSRC CCP5 Annual Meeting will be held in the School of Chemistry at The University of Birmingham from 6-8th September 1999.

The meeting will cover the traditional areas of CCP5, but with particular emphasis on applications of Monte Carlo, molecular dynamics and related techniques to the atomistic modelling and simulation of clusters (e.g. metallic and van der Waals clusters) and a wide range of interfacial systems (e.g. nanocolloids, micelles, solid surfaces, Langmuir-Blodgett films). The meeting will consist of invited and contributed oral presentations and there will be a poster session.

Invited speakers: Peter Coveney, Queen Mary and Westfield College, University of London; Julius Jellinek, Argonne National Laboratory, USA; Arthur F. Voter, Los Alamos National Laboratory, USA; David J. Wales, University of Cambridge.

ORGANISING COMMITTEE: Dr. Roy L. Johnston and Mrs. Lesley D. Lloyd, School of Chemistry, University of Birmingham, Tel. (44) 121 414 7477 (RLJ), Fax.(44) 121 414 4403, E-mail roy@tc.bham.ac.uk

Dr. John Harding Department of Physics & Astronomy, University College London E-mail j.harding@ucl.ac.uk

Dr. David Heyes, Department of Chemistry, School of Physical Sciences, University of Surrey E-mail d.heyes@surrey.ac.uk

Dr. Maurice Leslie CLRC Daresbury Laboratory, Daresbury E-mail m.leslie@dl.ac.uk

Conference timetable:

The meeting will start at 09.00 on Monday 6th September and finish at 13.00 on Wednesday 8th September. Accommodation is provided for the night of Sunday 5th September.

Registration and Accommodation:

A registration form is at the bottom of this email, and is also available at the CCP5 website (details given below). The full conference cost (including accommodation, meals and refreshments) is 150 pounds per person, reduced to 130 pounds for students. For those not requiring accommodation, the registration fee received before 1st August is 85 pounds, but is only 65 pounds for students. The registration fee covers lunches on Monday, Tuesday and Wednesday and the conference dinner on Tuesday 7th September.

There is a 20 pounds supplement for those registering after 1st August.

The accommodation fee is 65 pounds. Accommodation will be in University House, one of the student Halls of Residence, which is within a short walking distance of the School of Chemistry. The accommodation fee includes dinner on the evening of 6th September and breakfast on 6th, 7th and 8th. For anyone wishing to find their own accommodation, a list will be provided of nearby 'Bed & Breakfast' establishments and hotels.

Presentations and abstracts

An abstract should be sent (preferably at the time of registration and definitely before July 1st for oral presentations) by electronic mail in an electronic format, preferably in LATEX or simply as a text file. If you use MS WORD, please send the abstract as a rtf document. Oral contributions and posters are welcome.

The final date for submitting an abstract for an oral presentation is July 1st.

The final date for submitting an abstract for the poster session is August 1st.

The abstracts will also be published as part of an issue of the CCP5 quarterly newsletter. Delegates are also encouraged to submit a longer account of their work for publication in the newsletter. Postscript diagrams will also be accepted.

Travel Arrangements

Birmingham lies at the heart of England and can be reached easily by road, rail and air. The School of Chemistry is 5 minutes walk away from the University railway station (7 minutes from Birmingham New St. on the Birmingham to Longbridge or Redditch lines). University House is a further 10 minutes walk from the School of Chemistry. A taxi from the centre of Birmingham should cost around 7 pounds and a taxi from Birmingham International Airport should be around 15 pounds. Further information will be sent with the acknowledgement of registration.

25. JOHN P. SIMONS : A CELEBRATORY MEETING OF DYNAMICS AND SPECTROSCOPY

Oxford, 13 and 14 September 1999

A 2-day meeting is to take place in Oxford on 13 and 14 September 1999 to mark the retirement of John P. Simons as the Dr Lee's Professor of Physical Chemistry. The scientific sessions will be held in the Physical and Theoretical Chemistry Laboratory, with the conference being based on Trinity College. There will be 11 invited speakers and a few poster slots. More detailed information is available on the Web at <http://physchem.ox.ac.uk/meetings/jps>

26. MOLEC XIII (MOLEC 2000)

Jerusalem, Israel, September 17 - 22, 2000

The conference will be held at the 4-star hotel of Kibbutz Ramat Rachel, adjacent to Jerusalem. The social program will include sightseeing and an archeological tour of Jerusalem.

Local Organizing Committee:

Michael Baer (SOREQ Nuclear Research Center); Yehuda Band (Ben-Gurion University); Ronnie Kosloff (Hebrew University of Jerusalem); Assa Lifshitz (Hebrew University of Jerusalem); Nimrod Moiseyev (Haifa Technion); Abraham Nitzan (Tel Aviv University); Eli Pollak (Weizmann Institute Of Science); Salman Rosenwaks (Ben-Gurion University); Arlene Wilson-Gordon (Bar-Ilan University); Daniel Zajfman (Weizmann Institute of Science).

For more information contact M. Baer at Soreq Nuclear Research Center, Yavne 81800, Israel. email: mmbaer@netvision.net.il

Information also appears on the web (www.fh.huji.ac.il/~roib/MOLEC/index.htm)

Special announcement

INVITATION TO SUBMIT A PAPER

A special issue of **Physical Chemistry Chemical Physics** (a merger of the Journal of the Chemical Society Faraday Transactions and Berichte der Bunsen-Gesellschaft für Physikalische Chemie from Jan. 1999) on "MOLECULAR REACTION DYNAMICS: EXPERIMENT AND THEORY" will be published in 2000 to commemorate the scientific achievements of the late Roger Grice (1941-1998).

Editors: J.N.L. Connor, P.A. Gorry and J.C. Whitehead

Contributions in the form of regular papers are invited by 30 Sept. 1999

Further information from:

Professor J N L Connor,

Department of Chemistry,

University of Manchester,

Manchester M13 9PL, England.

e-mail: J.N.L.Connor@Manchester.ac.uk

BOOKS

Theory and Application of Quantum Molecular Dynamics

John Z.H. Zang, published by World Scientific

Detailed information on this book can be found at the following web sites:

<http://www.worldscientific.com/books/bookshop.html> (click on New Titles)

<http://p150.chem.nyu.edu> (click on Books)

The book can also be purchased from <http://www.amazon.com/>