

# Molecular Dynamics News

number 105; February 2000

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 has been accepted - otherwise state *unpublished*).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 106 to Prof. R. W. 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 (#105). The closing date for issue number 106 is April 1, 2000.

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\*2000 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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## 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. Subscribers may specify whether they want a raw LaTeX source file or a Postscript file.

### 2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file at the Molecular Dynamics News Web site: <http://www.ucsc.edu/mdn> A Web browser 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.

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 updated email and home page 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 more than 1600 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](mailto: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

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review molecular-dynamics-news
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to the address [mailbase@mailbase.ac.uk](mailto: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.**

## **a. Open Positions**

### **FACULTY**

#### **One Assistant Professor of Chemistry, Department of Chemistry University of Western Ontario London, Ontario Canada**

Analytical or Theoretical

The Department of Chemistry is inviting applications for a tenure track position at the rank of Assistant Professor in Analytical or Theoretical Chemistry. Applicants must have a Ph.D. degree or equivalent and suitable postdoctoral experience. The successful candidate will be expected to establish an independent, externally funded research program in their field of expertise and to participate with enthusiasm in teaching undergraduate and graduate courses in Chemistry. The Department of Chemistry ([www.uwo.ca/chem](http://www.uwo.ca/chem)) is a large, research intensive Department with strong programs in many areas of chemistry and with good interdisciplinary links to research groups in other Departments in the Faculties of Science, Engineering and Medicine and Dentistry.

Interested candidates should send their curriculum vitae, names of three referees along with a description of research accomplishments and a proposal for future research with an appropriate budget to Dr. D.H. Hunter, Department of Chemistry ([dhunter@julian.uwo.ca](mailto:dhunter@julian.uwo.ca)), The University of Western Ontario, London, Ontario, Canada, N6A 5B7. Phone: 519-661-3122, Fax: 519-661-3022 Closing date for receipt of applications is February 15, 2000.

In accordance with Canadian Immigration requirements, this advertisement is directed to Canadian citizens and immigrants of Canada. The University of Western Ontario is committed to employment equity, welcomes diversity in the workplace, and encourages applications from all qualified individuals including women, members of visible minorities, aboriginal persons and persons with disabilities. The position is subject to budget approval.

#### **Temple University, Faculty Positions in Physics**

The College of Science and Technology at Temple University is in the process of a major recruitment effort and is filling 34 faculty positions as part of a major expansion. The College invites applications for positions at the level of Full, Associate and Assistant Professor. Newly hired faculty will be given tenure track positions within the Department of Physics. Successful candidates are expected to have, or be able to develop, a significant research program supported by external funding and to have a strong commitment to teaching at both the undergraduate and graduate level. Candidates should also have a strong interest in interdisciplinary collaboration with the other Departments of the College as well as with Research Centers in the College, examples of which include the Center for Biotechnology, Center for Computer Science and Applied Mathematics, Center for Environmental Science and Technology, and the Center for Bioengineering and Biomaterials. In addition to these, new centers are being formed, including a center for advanced research in Physics to promote interdisciplinary collaboration.

Areas of particular interest include but are not limited to 1. high energy nuclear and particle physics, 2. soft condensed matter physics, and 3. molecular physics. Both experimentalists and theoreticians will be considered. Salary will be competitive and commensurate with qualifications and level of appointment.

Candidates should submit a letter of application, curriculum vitae, and a publication list, as well as evidence of teaching skills and a funded research program. They should also arrange to have three letters of reference sent to: Chair, Physics Faculty Search Committee, Office of the Dean, College of Science and Technology, 409 Barton Hall A, Temple University, Philadelphia, PA 19122. Additional information may be obtained at [www.temple.edu/physics](http://www.temple.edu/physics) or by e-mailing [meziani@vm.temple.edu](mailto:meziani@vm.temple.edu). Temple University is an Equal Opportunity/ Affirmative Action Employer.

Original announcement is available at:

[http://www.temple.edu/CST/jobs/Physics\\_ad\\_1999-2000.htm](http://www.temple.edu/CST/jobs/Physics_ad_1999-2000.htm)

### **Assistant Professor, Physical Chemistry, University of North Texas**

The Chemistry Department, University of North Texas, invites applications for a tenure-track Assistant Professor position from Ph.D. chemists with research interests in environmental chemistry.

Candidates must have a strong background in physical chemistry, and will be expected to conduct externally funded research, train doctoral students, and teach undergraduate and graduate physical chemistry courses. Interdisciplinary collaboration with faculty in Chemistry and the broader UNT community is encouraged. With an enrollment of over 26,000, UNT is the leading university in the growing Dallas-Fort Worth area. A full CV, statement of research plans and interests, and 3 recommendation letters should be sent to: Dr. Paul Marshall, Physical Chemistry Search Committee, University of North Texas, P.O. Box 305070, Denton, Texas 76203- 5070.

Further information: marshall@unt.edu or www.chem.unt.edu.

Applicant review begins Feb 1 and will continue until the position is filled. AA/ADA/EOE.

### **Professorship in molecular and optical physics, Lyon, France**

A professorship in molecular and optical physics is likely to become vacant at the Universite Claude Bernard, Lyon I (France), with a starting date October 2000.

The applicant will teach Optics, Laser Physics and Electromagnetism at undergraduate and postgraduate level.

The position will be associated with the Laboratoire de Spectrometrie Ionique et Moleculaire (LASIM) within the physics department. The laboratory wishes either to reinforce the existing molecular spectroscopy group of Professor J. d'Incan (retirement July 2000), using the high resolution Fourier transform spectrometry facility to work in atmospheric physics, or else to start a new independent research group in Optics, with interests in the non-linear properties of molecules at surfaces, in nanoparticles or aerosols. In the latter case, the new group will be expected to forge stronger links with the groups working on clusters, or on atmospheric pollution within the laboratory, and to interact with the nanotechnology projects of the physics department. Informal enquiries should be addressed to:

Professor Michel Broyer (Directeur du Laboratoire), Laboratoire de Spectrometrie Ionique et Moleculaire Batiment 205, Universite Claude Bernard Lyon I, Campus La Doua, 69622 Villeurbanne Cedex, FRANCE tel (33) 04 72 44 82 60, broyer@lasim.univ-lyon1.fr

or to Dr Christian Bordas, tel (33) 04 72 43 10 86, or to Dr Amanda Ross, tel (33) 04 72 44 85 63

REMINDER : Although this position will not be officially published until Spring 2000, the closing date for registration on the 'Liste de qualification aux fonctions de professeur aux universitas' has been set by the Ministere d'Education Nationale at 10th November 1999.

### **LECTURER (MAITRE-ASSISTANT) POSITION, UNIVERSITY OF LAUSANNE (SWITZERLAND)**

A lecturer (maitre-assistant) position is available immediately at the Institut de Physique de la Matiere Condensee-University of Lausanne. The candidate is expected to take part in teaching advanced physics courses to third and fourth (final) year students and/or basic physics to first year pharmacy and medical students. He or she will be involved in a research project using ultrafast laser spectroscopy to study photoinduced dynamics in condensed phase chemical systems and in biological molecules. The candidate should have a PhD in Physics or Physical Chemistry, along with at least two years of postdoctoral experience in the field of Ultrafast Spectroscopy. Knowledge of french language is highly recommended but not a condition. The base salary is approx. SFr. 80'000.- per annum. The University of Lausanne offers the possibility to do a habilitation.

Please send CV, list of publications and 2 Letters of recommendation to:

Prof. Majed CHERGUI, Vice-chair, Institut de Physique de la Matiere Condensee  
Faculte des Sciences BSP, Universite de Lausanne, Ch-1015 Lausanne, Switzerland  
tel.: xx-41-21-692 3678 (direct), (21) 692 3660 (secr.) Fax.:xx-41-21-692 3635, email:  
Majed.Chergui@ipmc.unil.ch <http://WWW.UNIL.CH/ipmc/>

## POST DOCTORAL AND VISITING

### **REACTION DYNAMICS Network - Postdoctoral opportunities**

A 4-year "research training network" (RTN) entitled: "REACTION DYNAMICS: EXPERIMENTAL AND THEORETICAL STUDIES ON THE DYNAMICS OF REACTIONS OF ATOMS AND RADICALS OF FUNDAMENTAL AND PRACTICAL IMPORTANCE" has recently been funded by the European Commission in the framework of the specific research and technological development programme "Improving the Human Research Potential and the Socio-economic Knowledge Base" (Fifth Framework Programme of the European Community). The network involves eight laboratories with contact people listed below.

The aim is to improve substantially our knowledge of the dynamics of elementary chemical reactions by combining, in a synergistic effort, state-of-the-art experimental techniques, based on molecular beam and laser spectroscopic methods, with state-of-the-art quantum chemical methods for calculating the potential energy surfaces that describe the reaction studied experimentally, and state-of-the-art quantum and quasiclassical methods for performing computations of scattering properties and thermal rate constants on these surfaces. Eight post-doctoral positions (for up to 3 years duration each) for young researchers with theoretical and/or experimental skills in the field of REACTION DYNAMICS will become available after March 1, 2000. Each group participating in the Network will soon advertise his own post-doc position. Informal inquiries are already welcomed at the addresses below.

Under the terms of the RTN programme, the young researcher applicants (aged 35 years or less) must be nationals of a Community Member State or a State associated with the RTN programme (Bulgaria, the Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia. Subject to its final conclusion, the Association Agreement signed with the Swiss Confederation is expected to enter into force on the 01.01.2001). The young researchers must not be nationals of the state in which the participant appointing them is established and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

Addresses of team leaders participating in the Network:

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universit di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

Dr. Mark Brouard, Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1 3QZ, UK, E-mail: mark.brouard@chemistry.ox.ac.uk (Phone: (+44) 1865-275457; FAX: (+44) 1865 275410).

Prof. J. J. Ter Meulen, Department of Applied Physics, University of Nijmegen, Toernooiveld 1, 6500 GL Nijmegen, The Netherlands, E-mail: htmeulen@sci.kun.nl (Phone: (+31) 24 365 3022; FAX: (+31) 24 365 3311).

Prof. P. Andresen, Fakultat fuer Physik, University of Bielefeld, Universitatstrasse 25, D-33501 Bielefeld, Germany, E-mail: andresen@physik.uni-bielefeld.de (Phone: (+49) 521 106 5450; FAX: (+49) 521 106 2958).

Prof. F. J. Aoiz, Departamento de Quimica Fisica I, Facultad de Ciencias Quimicas, Universidad Complutense de Madrid, Avenida Complutense s/n, 28040 Madrid, Spain, E-mail: aoiz@legendre.quim.ucm.es (Phone: (+34) 91 394 4126; FAX: (+34) 91 394 4135).

Dr. D. Manolopoulos, Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1, 3QZ, UK, E-mail: mano@physchem.ox.ac.uk (Phone: (+44) 1865-27545; FAX: (+44) 1865 275410).

Prof. H.-J. Werner, Institut for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany, E-mail: werner@theochem.uni-stuttgart.de (Phone: (+49) 711 685 4400; FAX: (+49) 711 685 4442).

Dr. U. Manthe, Institut of Theoretical Chemistry, Technische Universitatet Muenchen, Lichtenbergstrasse 4, 85747 Garching, Germany, E-mail: manthe@ch.tum.de (Phone: (+49) 89 289 13610; FAX: (+49) 89 289 28268).

## **POST-DOCTORAL POSITION AT EPA**

Chemical Physicist/Physical Chemist with experience in the use of laser-based spectroscopic methods for measurement of gaseous species. The ideal candidate will have hands-on experience with resonance enhanced multiphoton ionization (REMPI) or other laser spectroscopy of molecules. The candidate will work in an applied program that couples REMPI with time-of-flight mass spectrometry (TOFMS). The candidate will work with the leading international laser spectroscopy groups developing the REMPI analytical method and designing and building an instrument for use at EPA. Candidate will apply REMPI instrument for detection of trace halogenated air toxics as part of a comprehensive program at the EPA's combustion research facility in Research Triangle Park, NC, investigating the formation mechanisms of these pollutants.

### **Background**

The U.S. EPA's Office of Research and Development, National Risk Management Research Laboratory (Research Triangle Park, NC) conducts research on formation mechanisms, quantification methods, and prevention of hazardous air pollutants, particularly halogenated organics such as chlorinated dibenzodioxins/dibenzofurans, biphenyls, and naphthalenes. Recently, NRMRL has been awarded a grant to study the application of REMPI/TOFMS techniques toward development of a real time "dioxin" monitor. This grant program, combined with a DOE-funded program to develop the instrumental science behind REMPI/TOFMS, constitutes a large federally-funded effort whose goal is to develop this method of hazardous air pollutant detection for source characterization, understanding of pollutant formation mechanisms, and pollution prevention. As part of this program, a REMPI/TOFMS system will be built for use at EPA's combustion research facility. The post-doctoral laser spectroscopist is necessary to operate the REMPI/TOFMS system and develop its application for trace halogenated species detection. Candidate will work with a team of researchers investigating hazardous air pollutant formation on in-house facilities including waste combustors, industrial boilers, solid fuel combustors, rotary kilns, and laboratory reactors.

### **Particulars**

The optimal timing for arrival of this post-doctoral candidate is January-March, 2000. This timing will allow the candidate to work with the REMPI developer as they put together the instrument, allowing the candidate to better understand how the REMPI/TOFMS system works. Salary is US\$48,000 per year. This position is open to foreign nationals as well as U.S. citizens.

### **Information**

Further information can be obtained by contacting Dr. Brian Gullett, (919)541-1534, gullett.brian@epa.gov

## **Post-Doctoral Research Assistant University of Bristol, UK**

'SiO Maser Modelling - Assessment of Mass Loss and Hydrogen Concentrations in Late Type Stars'

Applications are invited for a post-doctoral position to work on a challenging project which seeks to investigate the rate of mass-loss from late type stars.

The candidate should have expertise in one or more of the following areas: 1) quantum-mechanical scattering theory; 2) ab-initio molecular electronic structure theory; 3) radiation transport and hydrodynamics. The project will use advanced techniques and computer codes from all these disciplines at different stages.

The objectives of the project will be to model the SiO maser radiation from the region of late type stars and from this modelling to ascertain the state and quantity of the hydrogen gas present in the region where mass-loss is initiated. This in turn will permit an estimation of the rate of mass loss from the stars involved. In order to model the maser radiation an improved knowledge of the vibrationally-rotationally inelastic collision cross sections of SiO with the most abundant available collision partners is needed. The project is already well under way and we have nearly finished the calculation of the necessary interaction potentials. The next stage of the project will be the computation of inelastic collision cross sections using these potentials followed by the use of the computed cross sections in maser modelling calculations.

The successful candidate will work with Prof. Gabriel Balint-Kurti (School of Chemistry), Dr. Malcolm Gray (Department of Physics and Astronomy, University of Wales, Cardiff) and Prof. David Field (Institute of Physics and Astronomy, Aarhus, Denmark). Applications should be made to Prof. G.G. Balint-Kurti (

School of Chemistry, University of Bristol, Bristol BS8 1TS, UK) and should supply the names of two referees.

Gabriel Balint-Kurti Gabriel.Balint-Kurti@bristol.ac.uk Tel: +44 (0)117 9287662 Fax: +44 (0)117 9251295  
<http://www.bris.ac.uk/Depts/Chemistry/staff/ggbk.htm>

### **POSTDOCTORAL FELLOWSHIPS IN ELECTRON and LASER SPECTROSCOPY IN THE DEPT. OF CHEMISTRY , SOUTHAMPTON UNIVERSITY**

Applications are invited for two postdoctoral fellowships, each to work for up to 3 years ,in the research group of Professor John Dyke.

Applicants should have a Ph.D in Chemistry or Physics.Experience in electron spectroscopy,molecular spectroscopy,vacuum technology or laser technology would be an advantage ,but is not essential. The first position is available from January 1st 2000,whilst the second position is available from September 1st 2000. The first post involves the study of reactivities intermediates using photoelectron spectroscopy with synchrotron radiation,and electron scattering, while the second position involves the study of radicals and molecular complexes with laser multiphoton ionization and related techniques.

Informal enquiries should be directed to Prof John Dyke at [jmdyke@soton.ac.uk](mailto:jmdyke@soton.ac.uk), or see <http://www.soton.ac.uk/~physchem.htm>

Prof. John M. Dyke, Dept. of Chemistry, The University, Southampton SO17 1BJ UK

Fax: +44 (0)1703 593781 Tel: +44 (0)1703 593590 Email: [jmdyke@soton.ac.uk](mailto:jmdyke@soton.ac.uk)

<http://www.soton.ac.uk/~chemweb/research/physchem.html>

### **Postdoctoral Research Position, University of Pittsburgh**

A Surface Probe Microscopy (STM/AFM) postdoctoral position is available in the Solid/Liquid Interface Group of the Surface Science Center at the University of Pittsburgh. The project is focused on the study of interface dynamics at the atomic and molecular level. Candidates should have previous experience with STM/AFM, especially in electrochemical environments. Experience with lasers and optics is a plus. The candidate should have strong problem solving skills, work well with others and demonstrate scientific leadership and initiative. As we also have Second Harmonic and Sum Frequency projects ongoing, this position is an excellent opportunity to learn more about linear and non linear optical probes of interfaces. The Surface Science Center at the University of Pittsburgh provides an excellent research environment. 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. Pittsburgh is safe, pleasant and affordable city offering the amenities of a major metropolitan area. 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.

Applications should be sent to: Dr. Eric BORGUET, Department of Chemistry and Surface Science Center, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh PA 15260, U.S.A.

(412) 624-8304 Office, (412) 624-8611 Fax

[borguet+@pitt.edu](mailto:borguet+@pitt.edu) <http://www.pitt.edu/~borguet/>

### **Postdoctoral position in ion-molecule reaction dynamics, University College London.**

A postdoctoral position is available in the Chemistry Department at UCL, from April 2000 for two years, to develop a new experiment to probe the dynamics of the bimolecular reactions of molecular doubly-charged cations. The considerable chemical reactivity of molecular dications has only recently been recognised, and little is known of the dynamics of the unusual chemical reactions they perform. The new experiment involves the application of a position-sensitive multi-coincidence technique [see J. Phys. B. 30, 4515 (1997) and J. Phys. B. 29, 5795 (1996)] to a bimolecular dication/neutral encounters and will allow the multiplex determination of the scattering diagram for the reaction under study. This project is part of a research programme at UCL, supervised by Dr. Stephen D. Price, which investigates the occurrence and consequences of multiple-ionization. The successful candidate will have completed a Doctorate in experimental physical

chemistry or chemical physics. Experience with time-of-flight mass spectrometry and high-vacuum techniques would be highly desirable.

Selected References: S. D. Price, *J. Chem. Soc. Faraday Trans.* 93, 2451 (1997). K. A. Newson and S. D. Price, *Chem. Phys. Lett.* 269, 93 (1997). K. A. Newson and S. D. Price, *Chem. Phys. Lett.* 294, 223 (1998). K. A. Newson, N. Tafadar, and S. D. Price, *J. Chem. Soc. Faraday Trans.* 94, 2735 (1998). N. Tafadar, N. Kaltsoyannis, and S. D. Price, *Int. J. Mass Spectrom.* 192, 205 (1999).

To apply: Please send a copy of a curriculum vitae and the names of three referees to:

Dr Stephen Price Department. of Chemistry University College London 20 Gordon Street London WC1H 0AJ. UK

Email: s.d.price@ucl.ac.uk Tel: +44 (0)20 7679 4606 <http://calcium.chem.ucl.ac.uk/webstuff/people/sdprice>

### **Postdoctoral Position, Concordia University, Quebec**

Post-Doctoral or Graduate Ph.D. Assistantship is available immediately in Theoretical/Computational (and possibly Experimental) Biochemistry. We are seeking outstanding candidates to investigate the role of proton transfer and hydrogen bonding in enzymatic reactions, as part of an international collaboration between various theoretical and experimental research groups at Concordia University and in France. The successful candidate will conduct theoretical research with Prof. Gilles H. Peslherbe (Concordia University, Montreal, Canada) and with Dr. James T. Hynes (at Ecole Normale Suprieure, Paris, France), primarily in connection with experiments performed at Concordia University in Prof. Ann English Laboratory. He/she may also have the opportunity to perform experimental research with Prof. Ann English. Applicants must be eligible for a Chateaubriand fellowship, which provides generous funding for studying one year in France. Interested and qualified candidates should contact Dr. Peslherbe immediately and/or send a complete Graduate School application to the Department of Chemistry and Biochemistry, Concordia University, 1455 De Maisonneuve Blvd West, Montreal, Quebec, CANADA H3G 1M8. Fax: (514) 848-2868. E-Mail: [ghp@alcor.concordia.ca](mailto:ghp@alcor.concordia.ca). For more information, see <http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe>

### **Institute of Atomic and Molecular Sciences, Academia Sinica Department of Physics, National Taiwan University**

Positions are open for POSTDOCS with Yuan T. Lee and Ralf I. Kaiser in the Institute of Atomic and Molecular Sciences (Academia Sinica) and the Department of Physics (National Taiwan University). We employ cutting edge crossed beams and matrix isolation techniques in the fields of material sciences, catalyses, combustion chemistry, and physical processes in interstellar environments and our solar system. The following research topics are available:

1. Formation and properties of boron and silicon bearing molecules relevant to semiconductor industry
2. Elementary mechanisms in 3d-group transition metal or zeolite catalyzed reactions (e.g. ices condensed on Fe, Ni, and Co layers)
3. Reaction dynamics in elementary processes in chemical vapor deposition (CVD) of carbon, boron, and silicon containing molecules
4. Formation of polycyclic aromatic hydrocarbon (PAH) molecules and soot in combustion processes and extraterrestrial environments
5. Synthesis of molecules in the gas phase or icy bodies in the interstellar medium or our solar system such as Jupiter, Saturn, Uranus, Neptune, Pluto, and especially Titan.
6. Synthesis of unstable radical intermediates in organic and metallo organic chemistry.
7. Formation of precursor molecules on proto Earth and extraterrestrial environments to biomolecules like carbon hydrates, DNA, and aminoacids.

Outstanding candidates with a high research commitment 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.iam.s.sinica.edu.tw](mailto:kaiser@po.iam.s.sinica.edu.tw).

### **Postdoctoral position, Department of Chemistry, Cambridge University**

A postdoctoral position is available immediately for three years to develop a new method to image channels and receptors on living cells. The method is a novel combination of scanning ion conductance microscopy

(see for example *Biophys. J.* 73,653-658 (1997)) with fluorescence microscopy . This is joint project between Dr David Klenerman ( Department of Chemistry, Cambridge University ) and Dr Yuri Korchev ( Department of Medicine, Imperial College, London). A good experimental background in scanning probe microscopy or fluorescence methods would be desirable but no prior knowledge of cell biology is required. To apply please send a copy of a curriculum vitae and the names of three referees to :

Dr David Klenerman, Dept Chemistry, Cambridge University, Lensfield Road, Cambridge CB2 1EW  
Email dk10012@cam.ac.uk Tel: 44-(0)1223-336481 Fax: 44-(0)1223-336362  
or

Dr Yuri Korchev, Imperial College School of Medicine, Division of Medicine, 5th floor MRC Clinical Sciences Centre, Hammersmith Campus, Du Cane Road, London W12 0NN  
Email: y.korchev@ic.ac.uk Tel.: 44(0)181 383 2362 Fax: 44(0)181 383 8306

### **Postdoctoral Position in Environmental Chemistry at SRI International**

The Molecular Physics Laboratory at SRI International has been awarded a Postdoctoral Fellowship by the Camille and Henry Dreyfus Foundation to employ a Ph.D. Chemist or Chemical Engineer to perform laboratory research in atmospheric chemistry.

Current research directions in our laboratory include experimental studies using Knudsen cell techniques and an aerosol flow reactor to address issues of stratospheric and tropospheric relevance. Choice of research topic will depend on the skills and interests of the postdoctoral scientist. Some areas of potential research are: heterogeneous chemistry on sulfuric acid surfaces heterogeneous chemistry on soot and/or mineral dust particles effect of trace metals in atmospheric particles role of iron catalysis in the reactions of organics in cloud and rainwater fate of biogenic emissions aqueous phase formation of multifunctional carboxylic acids

The postdoctoral researcher will play a large role in the development of some of the above activities.

Familiarity with vacuum techniques and mass spectrometry is desirable, as is experience with spectroscopy, chromatography, LabView programming, or chemical synthesis. The successful candidate will be chosen based on her/his chemical talents and commitment to environmental studies but is not expected to have prior training in atmospheric chemistry. Salary is competitive, and the Fellowship is renewable for a second year by mutual agreement of the Fellow, research supervisors, and the Dreyfus Foundation. Applications, including a curriculum vitae, selected publications and/or thesis abstract, statement of specific research interests, and at least two letters of recommendation should be sent to: David M. Golden or Laura T. Iraci, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave, Menlo Park, CA 94025. e-mail: golden@sri.com or laura.iraci@sri.com. (<http://www.sri.com/jobs/listings/32077.html>) Candidates are encouraged to apply by February 29, and review will continue until the position is filled.

### **Postdoctoral Positions, The Royal Institute of Technology, KTH, Stockholm**

The Goran Gustafsson POSTDOCTORAL FELLOWSHIP The Departments of Physics, Mathematics and Mechanics at the Royal Institute of Technology (KTH), Stockholm, Sweden, invites applications for one or two postdoctoral fellowships.

The successful candidate is expected to join an existing research group at one of the departments (mathematical, mechanics or physics) at the School. The duration of the stay is a minimum of 9 months and a maximum of 12 months, preferably beginning during the summer of 2000.

Candidates should submit, so as to arrive at KTH before March 1, 2000 a Curriculum Vitae (maximum 2 pages) and a list of publications, two or three letters of recommendation, including one from the research group of interest and a description of what work the candidate plans to perform at KTH (maximum 1 page). (Candidates cannot have their PhD degree from KTH or the Stockholm area.)

The stay at KTH must begin before September 1, 2000.

Applications should be sent to: Utbildningskansli DEF, KTH, S-100 44 STOCKHOLM, SWEDEN

Questions are preferably sent to any contact person you may have at the Departments of Mathematics, Mechanics or Physics. Please note reference number: 200-09-00

Information can also be found on the web: <http://www.atom.kth.se/~berg/pdoc.html>

Dr. Lars-Erik Berg, Director of Studies, Department of Physics, Royal Institute of Technology (KTH), S-10044 Stockholm, Sweden  
Phone: +46 8 7907124, FAX: +46 8 200430, e-mail: berg@atom.kth.se www.atom.kth.se/~berg/lasres.html

#### **Postdoctoral Position, Loughborough University**

A one year postdoctoral position is available, starting immediately, for 1 year on a European framework 5 project entitled "Study for the construction of a Quantum Information Processing Device using Doped Fullerenes". The work will involve using both classical dynamics and quantum (LDA) calculations on the structures of various doped fullerenes and their energetic interactions with different surfaces. Candidates should hold a Ph.D. or have equivalent research experience and have good computing and physical modelling skills. The salary will be 21,134 per annum for a start date of 1 March 1999.

Further information can be obtained from Professor Roger Smith, School of Mathematics and Physics, Loughborough University, Leicestershire, LE11 3TU, UK. (email: R.Smith@lboro.ac.uk)

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>

#### **Postdoctoral Fellow Position, University of British Columbia**

I have recently learned that I should shortly have funds available to hire a new postdoctoral fellow, starting pretty well immediately. I am looking for someone to do experiments in Fourier transform microwave spectroscopy of metal-containing systems, especially complexes and clusters prepared via laser ablation. We have two spectrometers (one currently being rebuilt to incorporate a mass spectrometer) available for the experiments.

I must emphasize that the work is primarily experimental, though willingness to do quantum chemical calculations to support the experiments would be helpful. But it is the experiments which count.

I would be grateful if anyone interested in this position would contact me at mgerry@chem.ubc.ca, and include a brief Curriculum Vitae, including the date of completion of doctoral requirements, and also names of referees.

Professor Michael Gerry, Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, B. C., Canada V6T 1Z1

Fax 1-604-822-2847

#### **Postdoctoral Position, University of Birmingham**

Applications are invited for a postdoctoral fellowship on a project in molecular reaction dynamics directed by Professor Ian W M Smith and Dr Ian R Sims. The research, including the postdoctoral position, is funded by EPSRC and the project is entitled:

The Formation and Reactions of Hydrogen in Specific Rovibrational States

The fellow will develop state-of-the-art laser methods for preparing and detecting H<sub>2</sub> in specific rovibrational levels. These methods will then be used to determine state-to-state information about bimolecular reactions in which H<sub>2</sub> is a reagent or product, including the rate constants for reaction H<sub>2</sub> with atomic and diatomic free radicals and the product state distributions of H<sub>2</sub> formed in the reactions of H atoms with vibrationally excited H<sub>2</sub>O and HCN.

The position is available from April 2000 for two years (one year renewable for a second). The exact starting date is negotiable. Applications are encouraged from candidates of any nationality.

Informal enquiries are welcome and should be directed to Professor Ian WM Smith FRS or to Dr Ian Sims.

This advert may also be found at <http://web.bham.ac.uk/i.r.sims/postdoc.htm>

Professor Ian W M Smith FRS, School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

Tel: +44 121 414 4422, Fax: +44 121 414 4426, Email: i.w.m.smith@bham.ac.uk

Dr Ian Sims, School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

Tel.: +44 (0)121 414 3782 Fax: +44 (0)121 414 4426 email: i.r.sims@bham.ac.uk  
<http://web.bham.ac.uk/i.r.sims/>

**Postdoctoral Position, International School for Advanced Studies in Trieste (Italy)**

A postdoctoral position is available, starting immediately, for 1 year on a project entitled:  
"Density-functional theory-based molecular dynamics simulations of biological systems"

The work will involve applications of the Car-Parrinello to systems of pharmaceutical relevance, such as targets for anti-AIDS and anti-cancer therapy.

For further information please send an email message to:

Dr. Paolo Carloni, International School for Advanced Studies, SISSA, via Beirut 4, 34014 Trieste, Italy

<http://www.sissa.it/cm/bc/>

email: carloni@sissa.it

Phone: +39-040-3787407, Fax:+39-040-3787528

**Postdoc position; Spectroscopy of semiconductor nanocrystals**

A postdoc position is available starting Spring 2000 in the group of Prof. Uri Banin, at the department of Physical Chemistry in the Hebrew University of Jerusalem, Israel.

The research topic is the size dependent optical spectroscopy of semiconductor nanocrystals and semiconductor cluster-molecules, which manifest the transition from the molecular regime to the solid state. the project is a collaboration with the group of Prof. Dr. Dieter Fenske from the Institute of Inorganic Chemistry in Karlsruhe, Germany. Interest and experience in optical spectroscopy methods, including cryogenic methods, is desired.

The position is offered for two years, extended on a yearly basis. Interested candidates should send further inquiries, a CV, list of publications, and have two letters of reference forwarded to Uri Banin at the address given below.

Some recent publications related to the proposed project are: U. Banin et. al, Nature 400, 542-544 (1999). M. Jacobsohn, U. Banin, J. Phys. Chem. B 104, 1-5 (2000). Y.W. Cao, U. Banin, Angew. Chem. Int. Ed. Eng. 38, 3692-3694 (1999).

Dr. Uri Banin, Department of Physical Chemistry, The Hebrew University, Jerusalem 91904, Israel  
TEL.:972-2-6584515, FAX: 972-2-5618033

**Postdoctoral Position, National Tsing Hua University, Taiwan**

A postdoctoral position in the area of gas-phase ultrafast reaction dynamics is available immediately at the Department of Chemistry, National Tsing Hua University, Taiwan. The postdoc will be expected to carry out experimental research based on femtosecond time-resolved photofragment translational spectroscopy, a relatively new and powerful technique in studying photodissociation dynamics. The experiments will use an amplified fsec Ti:sapphire laser system and a time-of-flight mass spectrometer operated under the energy-analyzing mode. The starting annual salary is about US24K. The initial appointment is for one year with the expectation of renewal for up to three years. Experience with ultrafast lasers and/or nsec laser-TOF-MS is desirable. Applicants should send a C.V. and arrange for at least two letters of recommendation to be sent to Prof. Po-Yuan Cheng, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 30043 (e-mail:pycheng@mx.nthu.edu.tw, FAX:886-3-571-1082)

**Postdoc positions: Theoretical/Computational Biophysics, SUNY Buffalo**

Postdoctoral positions are available after July 1, 2000 at Center for Single Molecular Biophysics of Department of Physiology and Biophysics of SUNY Buffalo to conduct theoretical and computational research in biophysics. Qualified candidates should have a PhD in Chemistry, Physics. The university Center for Computational Research also has 128-processor Origin 2000, 28-processor SP2, and a cluster of 64 Sun Ultra 5 workstations. Please send your CV with cover letter, and the names, addresses, and phone numbers of two referees familiar with your work. Email to zhou@tammy.harvard.edu with plain text file or postscript file is preferred. Regular mail should send to Dr. Yaoqi Zhou, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford St. 232, Cambridge, MA 02138, or Department of Physiology and

Biophysics, 124 Sherman Hall, University at Buffalo, State University of New York Buffalo, New York 14214 after July 1, 2000.

#### **Postdoctoral Position, Brookhaven National Laboratory**

A postdoctoral position is available in chemical dynamics involving thermal and photo-induced reactions of adsorbates on metal and metal-oxide surfaces. State-resolved probes of the desorbed products are used to study the charge and energy transfer processes induced by photoexcitation at the adsorbate-metal interface and the resulting reaction dynamics leading to desorption. This work is part of a larger interdisciplinary surface chemistry effort at Brookhaven which includes access to spectroscopy and structural beam lines at the National Synchrotron Light Source.

The successful candidate should have a background in laser-based chemical dynamics, surface (photo)chemistry or surface scattering. Experience with REMPI techniques, time-of-flight mass spectrometry or ion-imaging is also desirable. Brookhaven National Laboratory is an equal opportunity employer.

Applicants should send a CV and three letters of recommendation to: Michael G. White, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973 Phone: (516) 344-4345; e-mail: mgwhite@bnl.gov

#### **Postdoctoral Position, National Tsing Hua University, Taiwan**

A postdoctoral position in the area of gas-phase ultrafast reaction dynamics is available immediately at the Department of Chemistry, National Tsing Hua University, Taiwan. The postdoc will be expected to carry out experimental research based on femtosecond time-resolved photofragment translational spectroscopy, a relatively new and powerful technique in studying photodissociation dynamics. The experiments will use an amplified fsec Ti:sapphire laser system and a time-of-flight mass spectrometer operated under the energy-analyzing mode. The starting annual salary is about US24K. The initial appointment is for one year with the expectation of renewal for up to three years. Experience with ultrafast lasers and-or nsec laser-TOF-MS is desirable. Applicants should send a C.V. and arrange for at least two letters of recommendation to be sent to Prof. Po-Yuan Cheng, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 30043 (e-mail:pycheng@mx.nthu.edu.tw, FAX:886-3-571-1082)

#### **Postdoc Fellowship, Theoretical/Computational Chemistry, Taipei, Taiwan**

A postdoc fellowship in theoretical/computational chemistry is available in the molecular modelling lab of the Sun group at the chemistry department of the National Taiwan Normal University. The Department of Chemistry is one of the most research-active institutes in Taiwan. Our laboratory equipped with excellent computing resource provides an excellent environment for theoretical study of the condensed phases systems and molecular systems. The current topics include 'vibrational dynamics on semiconductor surfaces', 'protein backbone dynamics and unfolding', and 'face selectivity of reactions using quantum chemistry calculation'. Applicants with expertise in theoretical/computational chemistry area are welcome to send your CV and three reference letters to Ying-chieh Sun at sun@scc.ntnu.edu.tw, or the address: Department of Chemistry, National Taiwan Normal University, 88, Ting-Chow Road Sec. 4, Taipei, 11718, Taiwan, ROC Fax: 886-2-2932-4249 For more info, please look up <http://140.122.142.51/~sungroup>

The salary for this position is about 22,000 US dollars per year. Chinese is the language everybody speaks.

In the academic and research environment, there is no problem to communicate in English.

There are two channels for application of the postdoc positions. One is available immediately, the other is to apply these positions with applicant qualification and the projects he/she is going to work on. In the present case, I am going through the latter one this time at this moment of this fiscal year.

With the projects going on in my group and a suitable applicant's qualification, it is very much highly that the application will be approved if everything goes well. In this case, the postdoc fellowship will be available in about 3-4 months from the date of application.

#### **Postdoctoral position, Universite de Liege, Belgium**

A postdoctoral position is available for a period of twelve months starting around April 1, 2000 to investigate

the dynamics of unimolecular reactions in ion beams. Particular attention will be paid to kinetic (translational) energy release distributions. The research will be conducted both at the experimental and theoretical level but the balance between experimentation and theory will be determined by mutual agreement. For some of our recent publications, see J. Chem. Phys. 110, 2911 (1999); Int. J. Mass Spectrom. 185/186/187, 155(1999); J. Chem. Phys. 111, 9259 (1999). Salary will be equivalent to that offered to the university staff at the same level of qualification. Applications coming from graduate students will also be considered. Send applications and CV indicating previous experience to Prof. J.C. Lorquet, Departement de Chimie, Universite de Liege, Sart-Tilman, Batiment B6, Liege 1, Belgium; Fax: 32-04-3663414 or 32-04-3662933; e-mail: jc.lorquet@ulg.ac.be. Arrange for recommendation letters to be directly sent either by regular mail, fax or e-mail to the same address.

#### **DEPARTMENT OF CHEMISTRY, University of Southampton, UK**

An EPSRC funded postdoctoral position is available to work with Dr Richard Moss. The salary will be from £ 17570 and the starting date is as soon as convenient.

The title of this theoretical project is "Calculation of fully nonadiabatic properties of the hydrogen molecular cation and its isotopomers". It will involve analytical and computational quantum mechanics.

Further details of the project are at

<http://www.soton.ac.uk/~chemweb/jobs/physchem/remoss2.html>

and details of the Department may be found at <http://www.soton.ac.uk/~chemweb>

Dr Richard E Moss, Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK

Tel: +44 (0)23 80592193, FAX: +44 (0)23 80593781, email: [rem@soton.ac.uk](mailto:rem@soton.ac.uk)

www: <http://www.soton.ac.uk/~rem>

#### **POST DOCTORAL POSITION , University of Canterbury, New Zealand**

Post Doctoral position with Professor Peter Harland and Dr Robert Maclagan, Chemistry Department, University of Canterbury, Private Bag 4800, Christchurch, NEW ZEALAND.

A Marsden Fund (New Zealand Government) Post Doctoral position is available from 1st March 2000 for up to 24 months to investigate the dynamics of ion and electron collisions with spatially oriented molecules by crossed particle beams. Experience in experimental chemical physics, preferably involving crossed molecular beam studies, would be an advantage. A working knowledge of ultra-high vacuum systems, computer interfacing of instrumentation and techniques used for the measurement of small signals is essential. Preference will be given to candidates with experience in one or more of the following areas: charged particle studies; ion-imaging; instrument design; and computational chemistry.

The project leaders maintain collaborative links with international research groups including Rice University, The University of Georgia and The University of Oxford.

Salary \$NZD45,000 p.a. The average wage in New Zealand is \$NZ35,000. The cost of living in Christchurch is substantially lower than for the U.S. or Europe and the Post Doctoral salary will allow the appointee and family to live comfortably.

Christchurch is a city of 325,000 with excellent sporting and cultural opportunities. The Chemistry Department is recognised as one of the top Chemistry Departments in the Southern Hemisphere.

Information about the University is available on the web at <http://www.canterbury.ac.nz/> and

<http://www.canterbury.ac.nz/campusinfo/about/intro.htm>

Further information can be obtained from Professor Harland at the above address or

[p.harland@chem.canterbury.ac.nz](mailto:p.harland@chem.canterbury.ac.nz)

telephone: +64 3 364 2454 (Note that NZ time is GMT+12), fax: +64 3 364 2110

#### **NRC Postdoctoral Openings, Hanscom Air Force Base**

Two National Research Council Associate positions are available at the Air Force Research Laboratory at Hanscom Air Force Base, 15 miles northwest of Boston, Massachusetts. We perform laboratory research to better understand the chemistry and physics of the upper atmosphere. The research is conducted in an academic style and results are published in the open literature. U.S. citizenship is required for these positions, and applicants should be either soon-to-be or recent (past five years) PhD's. A modest-length

proposal, written with input from an AFRL staff member, is due 15 Jan 2000 together with supporting documents. The position is nominally for one year, with a second year of funding contingent on mutual interest. Salary is about \$45,000/year. See <http://national-academies.org/rap> for further details. We encourage submissions from motivated individuals, including those who wish to broaden their experimental knowledge base. Please contact the appropriate scientist (see below) for further information.

**Position 1:** Experiments in the COCHISE (COLD CHEMICAL Infrared Simulation Experiment) facility will be pursued, specifically: the spectroscopy and kinetics of excited nitrogen atom collisions with oxygen molecules [ $\text{fast N} + \text{O}_2 \rightarrow \text{NO}(v, \text{high } J) + \text{O}$ ] The details of the very highly rotationally excited product states of NO will be investigated as a function of precursor state. Metastable species will be monitored using spectrometric and interferometric detection of visible and IR emissions. Please contact Dr. Steven Miller at 781.377.2807 or [miller@plh.af.mil](mailto:miller@plh.af.mil) for further information.

**Position 2:** Experiments in the laser laboratory investigating energy transfer in key aeronomic processes will be pursued. Notably, these include vibrational energy transfer in collisions of NO and CO<sub>2</sub> with oxygen atoms. Laser techniques, including laser-induced fluorescence and transient diode laser absorption, will be used to detect the relevant species. Complex spectral and kinetic models will be developed to analyze and interpret the resultant data. Please contact Dr. Jim Dodd at 781.377.4190 or [dodd@plh.af.mil](mailto:dodd@plh.af.mil) for further information.

#### **NRC Postdoctoral Opening, Hanscom Air Force Base**

A National Research Council Associate position in theoretical Molecular Dynamics is available at the Air Force Research Laboratory (AFRL) at Hanscom Air Force Base, about 15 miles northwest of Boston, Massachusetts. We perform research to better understand the chemistry and physics of the non-equilibrium upper atmosphere. The research is conducted in an academic style and results are published in the open literature (See The Journal of Geophysical Research A, Geophysical Research Letters, and Chem. Phys. Lett. for our recent work). U.S. citizenship is required for this position, and applicants should be either soon-to-be or recent (past five years) PhD's. A modest-length proposal, written with input from an AFRL staff member, is due 15 Jan 2000 together with supporting documents. The position is nominally for one year, with a second year of funding contingent on mutual interest. Salary is about \$45,000/year. See <http://national-academies.org/rap> for further details. Please contact Dr. Ramesh Sharma at 781.377.4198 or [sharma@plh.af.mil](mailto:sharma@plh.af.mil) for further information.

#### **Postdoctoral position, Hebrew University of Jerusalem**

I am happy to announce an opening for a postdoctoral-position at the Hebrew University of Jerusalem, regarding Quantum Simulations of Proton Mobility and Acid Dissociation in water. This is a joint project with Prof. G.A. Voth, from the University of Utah, whose aim is to analyze in detail classical and quantum MD results obtained using the Utah MS-EVB/CMD software package, to elucidate the molecular mechanisms governing these fundamental processes.

Starting date: December 1999 in Jerusalem. Maximal duration – 3 years. A stay of several months in Salt Lake City during the year 2000 is anticipated. Fellowship is commensurate with regulations of the above Institutions and with candidate's qualifications, which should include: Good background in molecular dynamics, Fortran programming; Quantum calculations and parallel processing experience could be useful. Excellent/experienced Ph.D. candidates will also be considered. Kindly send updated CV, grades, list of publications and 2 letters of reference to:

Prof. Noam Agmon, Dept. Physical Chemistry, Givat-Ram Campus, The Hebrew University, Jerusalem 91904, ISRAEL

tel. 972-2-6585687, FAX 972-2-6513742, Email: [agmon@fh.huji.ac.il](mailto:agmon@fh.huji.ac.il)

Homepage: [www.fh.huji.ac.il/~agmon/index.html](http://www.fh.huji.ac.il/~agmon/index.html)

Relevant background publications by principal investigators: N. Agmon, Chem. Phys. Lett. 244, 456 (1995); J. Chim. Phys. (Paris) 93, 1714 (1996); J. Phys. Chem. A 102, 192 (1998); J. Molec. Liquids 73/74, 513 (1997). J. Lobaugh and G.A. Voth, J. Chem. Phys. 104, 2056 (1996); U.W. Schmitt and G.A. Voth, J. Phys. Chem. B 102, 5547 (1998). J. Chem. Phys. 111, 9361 (1999).

### **Postdoctoral position at Leeds**

A postdoctoral position is available in the femtosecond molecular dynamics group at Leeds University, UK. The project is focussed on the application of velocity map imaging (ion imaging) to Coulomb explosion pump-probe experiments on diatomic and triatomic molecules. A femtosecond laser is used to prepare an evolving wavepacket on a dissociative surface of the molecule. The time evolution is probed by the application of an intense ultra-short laser pulse ( $\sim 5\text{-}10$  mJ  $\sim 20$  fs) after a controlled delay. The intense pulse induces a Coulomb explosion in the molecule by stripping the valence electrons from the molecule. The ions are imaged using velocity mapping and thus the nuclear configuration at the moment of ionisation can be deduced.

The femtosecond molecular dynamics group provides an excellent research environment with a well equipped laboratory. The three permanent members of the group are Prof. Godfrey Beddard, Dr. Benjamin Whitaker and Dr. Gavin Reid. Currently there are three other members in the team. The laboratory is equipped with two amplified femtosecond lasers (home built) and a velocity mapping molecular beam apparatus. A Terahertz imaging system is also likely to be sited in the laboratory in the near future. Candidates should have strong experimental skills and the ability to work in a team environment. Experience of femtosecond laser systems would be an advantage but not essential given a strong background in chemical reaction dynamics or another area of chemical physics. The position is only open to non-UK European Union nationals (funding is through the EU TMR programme).

There are also openings for PhD students of any nationality.

Applications should be sent to:

Dr Benjamin J Whitaker, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK

tel: +44 113 233 6580, fax: +44 113 233 6565, web: <http://www.chem.leeds.ac.uk>

Further details about the TMR project can be found at <http://www.chem.leeds.ac.uk/IMAGINE>

### **Camille & Henry Dreyfus Postdoctoral Fellowship, Boston College**

A Camille & Henry Dreyfus Postdoctoral Fellowship is available to perform atmospheric chemistry laboratory studies in a joint program conducted in the Department of Chemistry at Boston College and at Aerodyne Research Inc. The research focuses on the heterogeneous interactions of atmospherically important gas phase species with liquids and with submicron aerosols, 40 to 1000 nm in diameter. Gas-liquid interactions are studied in droplet and bubble train apparatuses. Aerosol experiments are performed in a new apparatus that couples an aerosol sampling mass spectrometer with a fast flow reactor. The goal of the work is the study of chemical reactions of gas phase species with liquids and aerosols. The aerosol experiments are also designed to study changes in physical size and chemical composition of the aerosols after controlled exposure to reactive trace gases. The person in this position will participate in the on-going development of this novel apparatus as well as in the experimental studies. Experience in vacuum techniques and mass spectroscopy is desirable. This postdoctoral position presents an opportunity to be introduced to important aspects of atmospheric chemistry. Applicants should send their vita to Prof. Paul Davidovits, Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill MA 02467, e-mail: [paul.davidovits@bc.edu](mailto:paul.davidovits@bc.edu), Phone 617-552-3617. Boston College is an Equal Opportunity/Affirmative Action employer.

### **NRC Postdoctoral Opening, Hanscom Air Force Base**

The Space Chemistry group of the Air Force Research Laboratory Space Vehicles Directorate at Hanscom AFB, MA, is looking to fill an NRC post-doctoral research associate position. The successful candidate will conduct experimental research on ion processes using guided-ion beam and photodissociation techniques. Projects include the study of hyperthermal chemistry of atmospheric ions with small organic molecules, ion-metal vapor chemistry, inelastic and elastic scattering of atomic ions with atoms, photodissociation dynamics of small cluster ions, and the collision-induced dissociation dynamics of diatomic ions at high levels of vibrational excitation. The latter project is a collaborative effort with Prof. C. Y. Ng and involves prolonged assignments at the Lawrence Berkeley Advanced Light Source. The conducted research applies to modeling of extreme environments such as those of reentry vehicles, meteors, and electric propulsion

spacecraft thrusters.

The National Research Council (NRC) Resident Research Associateship Program provides highly qualified and motivated individuals AFRL on-site research assignments for one year, with second and third year extensions possible.

More information regarding the NRC associateship program can be obtained at the website, <http://www4.nationalacademies.org/osep/rap.nsf> or by calling Ms. Jacinta Kelly 202-334-1423.

Interested candidates should contact:

Rainer A. Dressler, Air Force Research Laboratory, AFRL/VSBS, 29 Randolph Rd, Hanscom AFB, MA 01731-3010

Tel: 781-377-2332, Fax: 781-377-8202, Email: [Dressler@plh.af.mil](mailto:Dressler@plh.af.mil)

World Wide Web: <http://www.plh.af.mil/Star/CPSE>

### **Postdoctoral Position, University of Utah**

A postdoc position is available in the lab of Scott Anderson, starting anytime after 1 January, 2000. The postdoc will work on our mode-selective ion-molecule reaction experiment, studying the reaction dynamics of simple polyatomic systems. We use REMPI and MATI ionization to prepare cations with variable excitation in selected vibrational modes, then study reactions in a high resolution guided-ion beam machine. The instrument also allows measurements of product velocity and angular distributions. Vibrational effects probe the early part of the collision, up to the point of initial "impact". The nature of the types of reactant motion (vibrational mode and relative energy) provide insight into the factors (e.g. transition state structure) that control reactivity and product branching. Angular distributions, coupled with isotope labeling, provide a measure of the timescale of the collisions, and how this varies with reactant energy and state. In direct reactions, the angular information allows us to distinguish between scattering mechanisms, and indirectly provides insight into the impact parameter dependence of the reactivity and product branching. Additional information can be found at my web site (see below) under the "State-selective Ion Chemistry" link.

Experience with pulsed laser spectroscopy and vacuum systems is desirable, however, I am most interested in working with a creative experimentalist. The initial appointment will be for one year, with the expectation of renewal for a second year contingent upon reasonable progress. 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 are encouraged. If interested, please send a C V and arrange for three letters of recommendation to be sent to: Scott L. Anderson, Professor of Chemistry, Dept. of Chemistry, 315 S. 1400 E., University of Utah, Salt Lake City, UT 84112-0850

(801) 585-7289, (801) 581-8433 FAX, [www.chem.utah.edu/chemistry/faculty/anderson/anderson.html](http://www.chem.utah.edu/chemistry/faculty/anderson/anderson.html)

### **Postdoctoral Research Associate, University of Surrey**

A 3-year Research-Council funded Postdoctoral Research Assistantship in Quantum Chemistry is available for work with Prof Graham A Webb and Dr Peter B Karadakov on the Ab Initio Calculation of Spectroscopic Parameters Relevant to the Determination of Carbohydrate Polymer Structures.

Applicants should have a PhD in theoretical chemistry or chemical physics; previous experience with ab initio codes such as GAUSSIAN and GAMESS is also desirable.

Starting salary will be on the RA1A scale in the range 16,286-19,869 per annum according to age and experience.

Further information can be obtained from:

Prof Graham A Webb (e-mail: [g.webb@surrey.ac.uk](mailto:g.webb@surrey.ac.uk)) or

Dr Peter B Karadakov (e-mail: [p.karadakov@surrey.ac.uk](mailto:p.karadakov@surrey.ac.uk))

Department of Chemistry, University of Surrey, Guildford, Surrey GU2 5XH, UK

tel +44 (0)1483 876828—fax +44 (0)1483 876851

Applications should be accompanied by a CV and the names and addresses of two referees.

### **POSTDOCTORAL POSITION, UNIVERSITY OF NORTH CAROLINA**

We are looking for a post-doc interested in moving into the emerging field of aerosol chemistry. This position will be joint between the research groups of Tom Baer and Roger Miller, on an AFOSR funded project dealing with the laser initiated combustion of single aerosol particles. The apparatus consists of a TOF laser-mass spectrometer into which we inject aerosol particles. These are detected by light scattering from two green diode lasers. This provides the triggering for a CO<sub>2</sub> laser, used to "ignite" the particles and for both a YAG pumped system and an excimer laser. The goal is to study the formation of radical intermediates during the liquid state combustion of these particles. A VUV laser is being developed to carry out near threshold ionization and H atom detection. REMPI and LIF is also available for state selective probing of the products, from which temperatures can be determined for the vapor plume. To date we have observed NO<sub>2</sub> elimination from nitrotoluene. We are now carrying out studies on higher energy molecules that can give rise to auto-catalytic processes.

This apparatus will also be used to determine compositions of atmospheric aerosols, related to the PM<sub>2.5</sub> issues. Ultimately we would like to develop methods that would enable us to depth profile such particles, providing detailed test of the molecules for organic aerosols and opening up a whole new range of uptake experiments.

The candidate need not have experience in aerosol science, but rather should have expertise in pulsed laser, TOF mass spectrometry.

Please send a cv and two letters of recommendation to: Tom Baer or Roger Miller, Chemistry Department, CB# 3290 Venable Hall, Chapel Hill, NC 27599-3290

### **POSTDOCTORAL POSITION, NATIONAL RESEARCH COUNCIL OF CANADA, OTTAWA**

We would like to hire a postdoctoral fellow in the area of theoretical molecular chemical physics. Experience in ab initio electronic structure calculations and/or variational and perturbative calculation of rotation-vibration energies would be an asset. We provide the successful applicant with a single node SGI 2000 workstation, and the Theory Group shares a 108 node SGI ORIGIN 2000.

Phil Bunker's research interests and recent publications can be viewed at <http://www.sao.nrc.ca/~bunker>

Application can be made by clicking on "NRC Post-Doctoral Fellowship" at the site

<http://hr.nrc.ca:8080/HRB/CareerPg.nsf/GradE>

If you apply please also contact [Philip.Bunker@nrc.ca](mailto:Philip.Bunker@nrc.ca)

### **POSTDOCTORAL POSITIONS, NATIONAL RESEARCH COUNCIL OF CANADA, OTTAWA**

Two postdoctoral positions are available in my group at the National Research Council in Ottawa.

We are currently pursuing theoretical research in several areas of molecular dynamics including:

- \* Gas-surface interactions: Control of surface reactions using a scanning tunneling microscope.
- \* Photomanipulation of external molecular modes: Molecular optics and molecular alignment with intense laser fields. [For recent publications in this area see: Phys. Rev. Lett. **83** (Dec. 6, 1999); J. Chem. Phys. **111**, 4397 (1999); J. Chem. Phys. **111**, 4113 (1999); J. Chem. Phys. **108**, 6272 (1998); J. Chem. Phys. **107**, 10429 (1997); Phys. Rev. A **56**, R17 (1997); J. Chem. Phys. **106**, 2881 (1997).]
- \* Time-resolved photoelectron spectroscopy as a probe of ultrafast, electronically nonadiabatic processes and of rotation-vibration coupling mechanisms. [Nature **401**, 5 (1999); J. Chem. Phys. **110**, 147 (1999); J. Chem. Phys. **107**, 7859 (1997).]
- \* Molecular interferometry in configuration space: The application of coherent control techniques to explore molecular continua. [J. Chem. Phys. **111**, 9168 (1999); Faraday. Discuss. **113**, 61 (1999); Accts. Chem. Res., **32** (Dec. 1999); Phys. Rev. Lett. **82**, 65 (1999); J. Chem. Phys. **108**, 1915 (1998); Phys. Rev. Lett. **79**, 4108 (1997).]

For more details and for abstracts of submitted papers and papers in press see: <http://gold.nrc.ca/~tamar> or contact me at: [tamar.seideman@nrc.ca](mailto:tamar.seideman@nrc.ca)

The Steacie Institute of the National Research Council offers multi-disciplinary research and a collaborative atmosphere. My group is lively and international and the computational facilities are excellent.

Applicants are asked to send me their Curriculum Vitae and to have two or more letters of recommendation sent to me directly, either by e-mail or by regular mail.

### **POSTDOCTORAL POSITION, University of Alberta**

A postdoctoral position is available in the group of Pierre-Nicholas Roy at the University of Alberta, Edmonton, Canada.

Research interests include the development of simulation methodologies for quantum molecular dynamics using path integral and semi-classical approaches.

Experience with classical and quantum molecular dynamics simulation methods is desirable. Candidates with a knowledge of parallel programming techniques are also strongly encouraged to apply.

Our computational resources include a 17 node PIII-500 Beowulf cluster and an IBM RS/6000 43P260 dual processor visualization workstation.

The starting date is early 2000 and the initial appointment is for a period of one year, renewable for another year (subject to the availability of funds).

Interested candidates should send a C.V., a summary of research interests and arrange for three letters of recommendation (email is ok) to be sent to Pierre-Nicholas Roy at the address below:

Professor Pierre-Nicholas Roy, Department of Chemistry, University of Alberta Edmonton, AB, Canada, T6G 2G2

tel: (780) 492-0317, fax: (780) 492-8231, email: pn.roy@ualberta.ca

www: <http://www.chem.ualberta.ca/faculty/Physical/roy.htm>

### **POSTDOCTORAL FELLOWSHIP, NATIONAL TSING HUA UNIVERSITY, TAIWAN**

One postdoctoral position starting January 2000 is open at the Department of Chemistry, National Tsing Hua University, Hsinchu, TAIWAN. The candidate is expected to be involved in the application of step-scan time-resolved Fourier-transform spectroscopy to gas phase absorption of transient species. This is a new technique with great potential. Please refer to J. Chem. Phys. **107**, 6499 (1997) for related articles. The appointment is renewable yearly with a salary about US\$24K plus housing. The tax is about 6% for those who stay more than 6 months in a calendar year. Applicants should send their c.v. and arrange 2-3 letters of recommendation to Prof. Yuan-Pern Lee, Department of Chemistry, National Tsing Hua University, TAIWAN 30043. (e-mail: [yplee@mx.nthu.edu.tw](mailto:yplee@mx.nthu.edu.tw), FAX: 886-3-5722892).

### **Postdoc Position, Hebrew University of Jerusalem**

A postdoctoral position is available in the group of Roi Baer at the Hebrew University of Jerusalem, Israel.

In our group, we are developing an exciting new approach to quantum chemistry, using a new Quantum Monte Carlo Technique called "Shifted Contour Auxiliary Field Quantum Monte Carlo". (See references at bottom). This work is made in collaboration with Daniel Neuhauser from UCLA.

The method is exciting because it alleviates the fixed node errors of other quantum Monte Carlo methods and it allows correlated sampling of energetical differences.

Our computational resources include a 85 node PIII-500 MOSIX cluster. The appropriate candidate should have a strong background in programming and theoretical chemistry. Preference to candidates with experience using plane wave methods and experience in programming in C++. The starting date is immediate and the initial appointment is for a period of one year, renewable for another year (subject to the availability of funds).

Interested candidates should send a C.V., a summary of research interests and arrange for three letters of recommendation (email is ok) to be sent to Roi Baer at the address below.

References:

- 1) R. Baer, M. Head-Gordon and D. Neuhauser, "Shifted-contour auxiliary field Monte Carlo for ab initio electronic structure: Straddling the sign problem" J. Chem. Phys. **109**, 6219 (1998).
- 2) R. Baer and D. Neuhauser, "Molecular electronic structure using auxiliary field Monte Carlo, plane waves and pseudopotentials" J. Chem. Phys. (in press, 1999).

Both reprints and a slide show can be viewed or downloaded from: <http://www.fh.huji.ac.il/~roib/qmc.htm>

Dr. Roi Baer, Dept. of Physical Chemistry and The Lise Meitner Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel  
Tel: 972-2-658-6114, Fax: 972-2-651-3742 email: roib@fh.huji.ac.il  
Web: <http://www.fh.huji.ac.il/~roib>

### **Postdoctoral Position, Korea Advanced Institute of Science and Technology**

We would like to control the branching ratio of the unimolecular dissociation of alkali dimers. The final goal would be the control of the reaction paths of bimolecular reactions. When the continuum is coupled with discrete states, asymmetric line profiles appear due to mutual interference. The product branching ratio can be changed abruptly along these asymmetric line profiles. We apply two coherent laser pulses and control the branching ratios by adjusting the relative phase between the two laser fields. In order to apply complex excitation scheme, appropriate excited states are searched.

Recent Ph. D's who have experience in laser spectroscopy and/or molecular beam are welcome. Our system is pulsed molecular beam of alkali metal dimers. We use Resonance Enhanced Multiphoton Ionization spectroscopy. Detection method by LIF would be utilized, too.

Theoreticians interested in ab initio calculation of alkali metal dimers can be considered for this position.

If you want more information please get to [http://www.chem.kaist.ac.kr/Bongsoo\\_Kim.html](http://www.chem.kaist.ac.kr/Bongsoo_Kim.html)

Professor Bongsoo Kim, Department of Chemistry, Korea Advanced Institute of Science and Technology, Taejeon, Korea

### **THREE POSTDOCTORAL POSITIONS, BROOKHAVEN NATIONAL LABORATORY**

The Gas-Phase Molecular Dynamics (GPMD) group in the Chemistry Department of Brookhaven National Laboratory, Upton, NY (USA) is a highly interactive, multidisciplinary team of researchers working on basic problems in spectroscopy, dynamics and kinetics related to obtaining a fundamental understanding of combustion processes at the molecular level (see <http://www.gpmd.bnl.gov>). The members of the group are:

James T. Muckerman (theoretical dynamics, spokesperson)

Trevor J. Sears (high-resolution absorption spectroscopy)

Gregory E. Hall (molecular dynamics using Doppler lineshape analysis)

Jack M. Preses (vibrational energy transfer)

Christopher Fockenberg (chemical kinetics).

Three postdoctoral positions are currently available for recent Ph.D.s: one in the area of theoretical/computational dynamics under the supervision of Dr. Muckerman; another in experimental chemical kinetics under the primary supervision of Dr. Fockenberg; and the other in experimental chemical dynamics under the supervision of Dr. Hall. The appointments are for one year, renewable for a second year, at an annual salary of approximately \$31,000. Brookhaven National Laboratory (BNL) is an equal opportunity employer, and US citizenship is not required.

The successful candidate for the theoretical/computational dynamics position should have a strong background in quantum dynamics and scattering theory, and will participate in computational studies of the vibrational structure of small hydrocarbon radicals, the calculation of rate constants for chemical reactions from the cumulative reaction probability, and laser control of molecular motion. One facet of this research involves the development of computer codes that make efficient use of massively parallel architectures.

The successful candidate for the experimental chemical kinetics position should have a strong background in chemical kinetics or chemical dynamics, and will participate in kinetics studies on radical-radical chemical reactions involving small hydrocarbon radicals using a new apparatus with TOF mass spectrometry as its primary detection technique. The research also includes investigations with a diode laser absorption system on selected reactions.

The successful candidate for the position in chemical dynamics should have a strong background in laser spectroscopy or chemical dynamics and will perform experiments using Doppler-resolved transient FM laser spectroscopy. In recent years our group has developed and applied this technique to a variety of problems in photoinitiated unimolecular reactions and direct photodissociation. We plan to extend previous work on correlated state distributions and fragment polarization in unimolecular reactions as an experimental probe of

the limits of validity for statistical theories of unimolecular reaction rates.

Applicants should submit a CV with a list of publications, a brief statement of research interest, and three letters of recommendation. Send all correspondence to:

James T. Muckerman (Email: muckerma@bnl.gov ), or Christopher Fockenber (Email: fknberg@bnl.gov ), or Gregory E. Hall (Email: greghall@bnl.gov )

Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

### **Postdoctoral Position, National Research Council, Ottawa**

A joint postdoctoral position in the area of time-resolved dynamics is available in the groups of Tamar Seideman and Albert Stolow at the Steacie Institute for Molecular Sciences of the National Research Council of Canada.

We are particularly interested in nonadiabatic dynamics in polyatomic systems as viewed by time-resolved photoelectron angular and energy distributions. The successful candidate will carry out theoretical work in the group of Tamar Seideman in direct collaboration with the experimental group of Albert Stolow.

Relevant recent Publications include:

- 1) V. Blanchet, M. Zgierski, T. Seideman and A. Stolow, "Discerning Vibronic Molecular Dynamics via Time Resolved Photoelectron Spectroscopy", *Nature* **401**, 52 (1999).
- 2) S.C. Althorpe and T. Seideman, "Molecular Alignment from Femtosecond Time-Resolved Photoelectron Angular Distributions: Non Perturbative Calculations on NO", *J. Chem. Phys.* **110**, 147 (1999).
- 3) V. Blanchet A. Stolow, "Nonadiabatic Dynamics in Polyatomic Systems Studied by Femtosecond Time-Resolved Photoelectron Spectroscopy", *J. Chem. Phys.* **108**, 4371 (1998).
- 4) T. Seideman, "Time-Resolved Photoelectron Angular Distributions: A Nonperturbative Theory", *J. Chem. Phys.* **107**, 7859 (1997).

For more details see:

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

[http://gold.sao.nrc.ca/sims/femto\\_e.html](http://gold.sao.nrc.ca/sims/femto_e.html)

Or contact us at: tamar.seideman@nrc.ca or albert.stolow@nrc.ca

### **Postdoctoral Position, Concordia University**

A postdoctoral position is available immediately in Computational and Theoretical Chemistry in the Department of Chemistry and Biochemistry at Concordia University. The successful candidate will be involved in various components of our research program, including studies of novel cluster materials and catalysts, cluster and liquid solvation in photochemistry, proton transfer and role of hydrogen bonding in biological systems. Preference will be given to candidates with a strong background in traditional, Car-Parrinello and QM/MM Molecular Dynamics Simulations, and/or Electronic Structure Calculations. Solid programming ability a plus. Salary commensurate with experience. Fax, mail or e-mail letter of intent and resume, and have three reference letters sent to Prof. Gilles H. Peslherbe, Department of Chemistry and Biochemistry, Concordia University, 1455 De Maisonneuve Blvd West, Montreal, Quebec, CANADA H3G 1M8. Fax: (514) 848-2868. E-Mail: ghp@alcor.concordia.ca. More information can be found at <http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe>.

Professor Gilles H. Peslherbe, Concordia University, Department of Chemistry and Biochemistry, 1455 De Maisonneuve Blvd Ouest, Montreal, Quebec, CANADA H3G 1M8

Tel: (514) 848-3335, Lab: (514) 848-3336, Fax: (514) 848-2868, E-Mail: ghp@alcor.concordia.ca

<http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe>

### **Postdoctoral Research Assistantship, University of Bristol**

Applications are invited for a Postdoctoral Research Assistantship to work for up to 2 years with Dr Colin Western on the development of a novel, very high resolution, all solid state pulsed laser system and its application to the spectroscopy and dynamics of molecular systems. Applicants should have a PhD in either Chemistry or Physics. The position, which would particularly suit persons with a background in laser development or laser spectroscopy is available from 1 April 2000. Salary will be on the RA1A scale, currently in the range £16,286 - £18,185 pa.

Informal enquiries should be directed to: C.M.Western@bristol.ac.uk or see:

<http://www.chm.bris.ac.uk/pt/western/vac2.htm>

For further details telephone (0117) 954 6947, minicom (0117) 928 8894 or E-mail Recruitment@bris.ac.uk quoting reference 6046. Applications, which should include a CV and the names of two referees, must be sent to the Personnel Office University of Bristol, Senate House, Bristol BS8 1TH by the 21 Jan 2000.

### **POSTDOCTORAL POSITION, BROOKHAVEN NATIONAL LABORATORY**

A postdoctoral position is available in chemical dynamics involving thermal and photo-induced reactions of adsorbates on metal and metal-oxide surfaces.

State-resolved probes of the desorbed products are used to study the charge and energy transfer processes induced by photoexcitation at the adsorbate-metal interface and the resulting reaction dynamics leading to desorption. Current and future projects include fundamental studies of photodesorption, UV and IR-induced recombination and association reactions, surface reaction kinetics and molecular beam scattering. This work is part of a larger interdisciplinary surface chemistry effort at BNL which includes access to spectroscopy and structural beam lines at the National Synchrotron Light Source.

The successful candidate should have a strong background in laser-based chemical dynamics, surface (photo)chemistry or surface scattering. Experience with REMPI techniques, time-of-flight mass spectrometry or ion-imaging is also desirable. Brookhaven National Laboratory is an equal opportunity employer, and US citizenship is not required.

Applicants should send a CV and three letters of recommendation to:

Michael G. White, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973

ph: (516) 344-4345, fax: (516) 344-5815, e-mail: mgwhite@bnl.gov

### **POSTDOCTORAL POSITION, UNIVERSITY OF PERUGIA**

Applications are invited for a postdoctoral fellowship in Astrophysical Chemistry under the supervision of Professor Piergiorgio Casavecchia, and funded by the European Union's TMR (Training and Mobility of Researchers) Programme, as part of the TMR Network on "Astrophysical Chemistry: Experiments, Calculations, and Astrophysical Consequences of Reactions at Low Temperatures". This programme involves eight laboratories: University of Birmingham (UK), University College London (UK), University of Goettingen (Germany), Technische Universitat Chemnitz (Germany), University of Rennes (France), Observatoire de Paris, Meudon (France), University of Bordeaux (France), and the University of Perugia (Italy).

The focus in our laboratory is on studies of chemical reaction dynamics using the Crossed Molecular Beams scattering technique with universal mass-spectrometric detection. Investigation of elementary atom(radical)-molecule and atom-radical reactions of relevance to Astrochemistry are being pursued. We exploit the novel capability of generating intense and continuous supersonic beams of carbon and nitrogen atoms, and hydroxyl (OH) and cyano (CN) radicals. All these beams have already been successfully tested and used for experiments. Experiments are planned on N, C, and CN reactions, as well as on atom-radical reactions as N+OH. More details of the research field, the technique used, and publications may be found at the following site: <http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html> and details of the Astrophysical Chemistry TMR Network should also be consulted: <http://www.bham.ac.uk/Astrochemistry/> The position is available from January 2000 for one year (actually 13 months). The exact commencement date is negotiable. The post-doc is expected to spend up to one month each year in another laboratory of the TMR network. Salary is about 3000 EURO/month. Under the terms of the TMR Programme, applicants

must be nationals of a Community Member State or a State associated with the TMR Programme (Iceland, Israel, Liechtenstein, Norway). The young researchers must not be nationals of the state in which the participant appointing them is established (i.e., Italy) and must not have carried out their normal activities in that state for more than 18 of the 24 months prior to their appointment. Experience in reaction dynamics and molecular beams is desirable.

Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcomed. Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

## b. Preprints

### **The He + H<sub>2</sub><sup>+</sup> reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern**

Chem. Phys. Lett., 318, 619-628 (2000)

V. Aquilanti, G. Capecchi, S. Cavalli, D. De Fazio

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

P. Palmieri, C. Puzzarini

Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, 40126 Bologna, Italy

A. Aguilar, X. Giménez, J.M. Lucas

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

Quantum mechanical calculations on three potential energy surfaces for the prototype ion-molecule reaction He + H<sub>2</sub><sup>+</sup> → HeH<sup>+</sup> + H have been performed in order to test the influence of their accuracies on reaction probabilities and cross sections.

### **Harmonic analysis and discrete polynomials. From semiclassical angular momentum theory to the hyperquantization algorithm**

Theor. Chem. Acc.

V. Aquilanti, G. Capecchi

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

Orthogonal polynomials of a discrete variable have been widely investigated as fundamental tools of numerical analysis. This work aims to propose to extend their use to quantum mechanical problems.

### **Reactions of C<sup>+</sup>(<sup>2</sup>P<sub>j</sub>) with CO(<sup>1</sup>Σ<sup>+</sup>) from thermal energies to 30 eV**

J. Chem. Phys. Wenyun Lu, Paolo Tosi, Mauro Filippi, and Davide Bassi

INFN and Dipartimento di Fisica, Università degli Studi di Trento, I-38050 Povo - Italy

### **The reaction N<sub>2</sub><sup>+</sup> + N<sub>2</sub> → N<sub>3</sub><sup>+</sup> + N from thermal to 25 eV**

Paolo Tosi, Wenyun Lu and Davide Bassi

INFN and Dipartimento di Fisica, Università degli Studi di Trento, I-38050 Povo, Italy

### **Bond-forming reactions of molecular dications with rare gas atoms. Production of ArC<sub>2</sub><sup>+</sup> in the reaction CO<sub>2</sub><sup>+</sup> + Ar**

Wenyun Lu, Paolo Tosi, and Davide Bassi

INFN and Dipartimento di Fisica, Università degli Studi di Trento, I-38050 Povo, Italy

### **Gauge symmetry, chirality and parity violation in four-particle systems: Coulomb's law as a universal molecular function**

Authors: G. Van Hooydonk

Comments: 90 p., 5 tables, 35 figures

Report-no: CB00-01

Subj-class: General Physics; Chemical Physics

Following recent work in search of a universal function (Van Hooydonk, Eur J Inorg Chem, 1999, 1617), we test symmetric potentials for reproducing molecular potential energy curves (PECs). For a bond, four-particle system, charge inversion is the key to explain this shape generically. A parity adapted Hamiltonian reduces from ten to two terms. The analytical perturbed Coulomb function scales attractive and repulsive branches of 13 PECs (HH, HF, LiH, KH, AuH, LiLi, LiF, KLi, NaCs, RbRb, RbCs, CsCs and II) in a single straight line. Turning points are reproduced with a deviation of 0.3 the repulsive side, the deviation is 0.2 molecular parameter function gives PECs of acceptable quality, just using atomic ionisation energies. The function can be used as a model potential for inverting energy levels. The theory may be tested with femtochemistry. Reactions between hydrogen and anti-hydrogen, feasible in the near future, will probably produce normal HH.

### **Multiphoton Ionization of Inner-Valence Electrons and Fragmentation of Ethylene in an Intense Laser Pulse**

Chemical Physics Lett. 313,789-794(1999)

A Talebpour, A.D. Bandrauk, S.L. Chin

Dept de Physique & Laboratoire de Chimie Theorique

Universite Laval & Universite de Sherbrooke, Que, Canada

Linearly polarized 200 fs Ti-sapphire laser pulses are used to study ionization and fragmentation of ethylene at high intensities. A model is proposed to explain the production of different fragments,  $C_2H_4^+$ ,  $C_2H_3^+$  and  $C_2H_2^+$  as a function of Intensity.

### **Laser Pulse Control of Raman Processes by Chirped Non-Adiabatic Passage-CNAP.**

F. Legare, S. Chelkowski, A.D. Bandrauk

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

Chirped pulses allow for non-adiabatic passage between dressed states of Raman processes. It is shown by numerical simulation that an appropriately chirped pulse can control the interference between resonant and non-resonant pathways in stimulated Raman processes.

## **c. Conferences**

### **1. Astrophysical Chemistry Group Young Researchers Meeting**

Monday 6th March 2000, Burlington House, London, 11am-5pm

Wine reception at the RAS 5-6pm

DEADLINE FOR REGISTRATION 31st JANUARY 2000

DEADLINE FOR RECEIPT OF ABSTRACTS 31st JANUARY 2000

The Astrophysical Chemistry Group of the Royal Society of Chemistry and the Royal Astronomical Society is arranging a one-day meeting aimed primarily at PhD students and also postdocs. The meeting will cover many different facets of this rapidly expanding research area, from observational work in all regions of the spectrum, through theoretical modelling, to laboratory data.

The number of places at the "Expanding Your Universe" meeting is limited to 50, and places are being allocated on a first come first served basis consistent with producing a balanced programme. Over 40 applications have already been received, from PhD Students, Postdoc's, Lecturers and Professors from the U.K. and Europe.

We look forward to seeing you all in March! Please visit our website

<http://www.nottingham.ac.uk/~pczhjf/astrochem.htm>

for further information and do not hesitate to contact Dr. Fraser if you have further questions.

Dr. Helen Jane Fraser

Department of Physical Chemistry

University of Nottingham

University Park

Nottingham

NG7 2RD

tel:0115 951 3472

fax:0115 951 3562

helen.fraser@nottingham.ac.uk

## **2. CONDENSED MATTER DIVISION, EUROPEAN PHYSICAL SOCIETY**

Montreux, Switzerland, March 13 to 17, 2000

The next (18-th) General Conference of the Condensed Matter Division of the European Physical Society will be held in Montreux, Switzerland from March 13 to 17, 2000, jointly with the Japanese and the Swiss Physical Societies (see <http://www.eps-cmd18.ch> for details). The Conference consists of plenary sessions, parallel sessions and 1/2 day mini-colloquia on specialised topics. A mini-colloquium (see abstract below) will be organized on

### **ULTRAFAST SPECTROSCOPY OF CONDENSED MATTER**

and will contain invited talks, contributed oral presentations and poster presentations.

The invited speakers are:

Jochen FELDMANN, Univ. Muenchen, Germany

Soren KEIDING, Univ. of Aarhus, Denmark

Takayoshi KOBAYASHI, Univ. of Tokyo, Japan

We strongly encourage you to submit abstracts for contributed papers and for posters. Abstracts should be submitted via the Web page of the conference <http://www.eps-cmd18.ch> before November 15th, 1999.

Please fax or email a copy to M. Chergui (see address below).

**IMPORTANT DEADLINES:** 15 November 1999 Abstract submission

31 January 2000 Conference registration

21 February 2000 Hotel registration

M. Chergui, V. Sundstrom ([Villy.Sundstrom@chemphys.lu.se](mailto:Villy.Sundstrom@chemphys.lu.se)) Chairs of the mini-colloquium

### **MINI-COLLOQUIUM ON ULTRAFAST SPECTROSCOPY OF CONDENSED MATTER**

The scope of the mini-colloquium is to present the most recent scientific and technological developments in the field of ultrafast spectroscopy. In addition to the traditional condensed matter systems which are being investigated by ultrafast spectroscopy (e.g. semi-conductors), ultrafast phenomena in many body systems such as clusters, solutions, surfaces and interfaces, molecular solids and biological systems will be covered.

The phenomena of interest include carrier dynamics, structural dynamics, energy dissipation, energy transfer, electron dynamics, chemical dynamics and solvent dynamics. From the technological point of view, the development of new ultrashort light sources from the IR to the X-ray domain will be covered, as well as new experimental techniques for the study of condensed matter. The mini-colloquium will include 3 invited talks, 6 to 8 contributed talks and a 2-hour poster session.

## **3. Gas Kinetics Group Winter Meeting**

Royal Society of Chemistry, Faraday Division Gas Kinetics Discussion Group

Winter Meeting, March 21st - 22nd, 2000, University of Reading

The annual winter meeting of the Gas Kinetics Group will be held from early afternoon on Tuesday March 21st to late afternoon on Wednesday March 22nd, 2000 in the Department of Chemistry, University of Reading.

The theme of the meeting will be atmospheric chemistry. The speakers are drawn from participants in the NERC-sponsored Laboratory Studies in Atmospheric Chemistry (LSAC) and Instruments for Field Measurements in the Atmosphere (IFMA) programmes. Additional poster contributions on any broadly related topic are invited.

Invited lectures will include:

M J Pilling Reactions of alkoxy radicals

I W M Smith Low temperature kinetic measurements relevant to the stratosphere

D M Rowley, A Cox Laboratory studies of gas-phase bromine and iodine chemistry

H-L Windsor, R Toumi Fractal fluctuation of pollutant concentrations

P Brimblecombe, S L Clegg, M Massucci The electrolyte thermodynamics of liquid droplets in the atmosphere

G Hancock Recent developments in the photochemistry of ozone

A J Orr-Ewing Applications of cavity ring-down spectroscopy to atmospheric chemistry

J M C Plane Meteoric materials in the upper atmosphere

A Horn IR spectroscopy applied to heterogeneous atmospheric catalysis

G V Buxton, M Bydder, G A Salmon, J E Williams, F Wilkinson The influence of cloud on atmospheric chemistry

H K Roscoe, J Pyle, N Harris IFMA in the atmosphere - tracers, reservoirs and radicals

D E Heard, M J Pilling Field measurements of OH and HO<sub>2</sub> radicals

I M Povey, A M South, C Hill, E G Norton, R L Jones Broadband lidar measurements of tropospheric constituent profiles and their atmospheric implications

A Illingworth, R Hogan, J Eastman Dopplerisation of a 94 GHz cloud radar

P Kaye, R Greenaway, E Hirst, J Barton, D Secker Spatial light scattering for aerosol and atmospheric cloud particle characterisation

Please print off, edit and return the accompanying form (hard copies have been sent to existing Group members), or send the equivalent information via e-mail, to the Local Organiser:

Dr. George Marston Department of Chemistry, University of Reading Whiteknights, PO Box 224, Reading RG6 6AD e-mail: G.Marston@reading.ac.uk

by the closing date of 31st January, 2000.

Further details of the programme and arrangements will be sent to those who register.

Gas Kinetics Group Meeting

March 21st - 22nd, 2000, University of Reading

Registration Form

Title / Name.....

Address and Affiliation

.....

.....

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.....

Phone:.....FAX:.....

E-mail.....

I would like to present a poster: YES / NO

Title:

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.....

.....

Authors:

.....

.....

Registration and Meals

Inclusive charge for registration, conference dinner on 21st March, lunch on 22nd March, teas and coffees, etc.

Full rate: 80

Reduced rate for postgraduate students: 55

(requires signature of supervisor

.....)

Please specify any special dietary requirements:

.....

Accommodation for the night of 21st March: 26

Accommodation for additional nights: 26 per night

(Please specify : 20th March / 22nd March)

Enter Total remittance:

Please specify method of payment:

(cheques made payable to The University of Reading)

enclosed / sent separately / other .....

.....)

Return by 31st Jan. 2000 to:

Dr. George Marston, Department of Chemistry, University of Reading, Whiteknights, PO Box 224, Reading RG6 6AD or e-mail: G.Marston@reading.ac.uk

Dr. K. G. McKendrick, Secretary, Gas Kinetics Discussion Group, Department of Chemistry, The University of Edinburgh, King's Buildings, Edinburgh EH9 3JJ, UK

Tel: -44-131-650 4735, FAX: -44-131-650 4743

#### **4. FARADAY DISCUSSION 115 - MOLECULAR PHOTOIONISATION**

3-5 April 2000, University of York, UK

Closing date for application forms:

Early Bird Closing Date: Friday 28 January 2000

Standard Closing Date: Friday 25 February 2000

Download the second circular, registration form and application form for student bursaries from the FD115 home page

<http://www.rsc.org/lap/confs/fara115.htm>

#### **INTRODUCTION**

Molecular photoionisation dynamics presents a challenge both from experiment and theory. New insight has come from the development and application of (i) novel experimental techniques, such as ZEKE and related pulsed-field ionization spectroscopies, anion photodetachment, time-resolved probing, angular photoelectron measurements, advanced coincidence techniques and (ii) new theoretical approaches to quantitatively understand the ionisation dynamics. There is an interest in advancing this burgeoning field and very actively studied applications come from van der Waals and hydrogen bonded molecular clusters including intra-cluster reactions, molecular Rydberg states including their time-resolved dynamics and their stability in fields, Multichannel Quantum Defect and scattering theory, Rydberg state tagging, molecular and cluster anion photodetachment, radicals, charge

The Discussion is intended to bring together practitioners of the broadest range of photoionisation, photodetachment and charge transfer experiments, spectroscopists, molecular physicists and theoreticians working on angular momentum transfer, scattering theory, electron correlation and on non-Born-Oppenheimer effects in Rydberg states. The aim is to establish state-of-the-art applications in chemistry and molecular physics, while focussing on the immediate future prospects of this whole area of research.

Professor Klaus Miller-Dethlefs, Chairman, Faraday Discussion 115, University of York, UK

#### **PROGRAMME**

The Discussion will comprise 4 sessions and a poster session, the first session commencing after lunch on Monday 3 April 2000, and the final session ending at lunchtime on Wednesday 5 April 2000. The papers listed below will be presented and discussed during the course of the meeting although not necessarily in the stated order. The time at which each paper will be given will depend on their grouping and on the length of the discussion periods.

**THE PRESIDENT:** Professor Sir John Meurig Thomas CChem FRSC FRSE FRS

**PROVISIONAL Monday 3 April 2000 Session 1: 14.00 - 18:00 hrs SESSION TIMES: POSTER SESSION 19.30 hrs**

**Tuesday 4 April 2000 Session 2: 09.00 - 12.30 hrs Session 3: 13.30 - 17.30 hrs**

**Wednesday 5 April 2000 Session 4: 09.00 13.00 hrs**

**INTRODUCTORY LECTURE:**

Probing Wavepacket Dynamics with Femtosecond Energy - and Angle-resolved Photoelectron Spectra K Takatsuka and Y Arasaki, University of Tokyo, Japan, and K Wang and B V McKoy, California Institute of Technology, Pasadena, USA

Towards Disentangling Coupled Electronic-vibrational Dynamics in Ultrafast Non-adiabatic Processes V Blanchet, M Z Zgierski, T Seideman, Z-C Yan, S Lochbrunner, J J Larsen, M Schmitt, J P Shaffer and A Stolow, Steacie Institute for Molecular Sciences, Ottawa, Canada

Time-resolved Studies of Electron Solvation Dynamics in Clusters D Neumark, University of California, Berkeley, USA

Time-and-Frequency-resolved Photoelectron Spectroscopy of the Allyl Radical:  $C_3H_5$  and  $C_3D_5$  T Schultz, T Gilbert and I Fischer, ETH Zurich, Switzerland

Bound and Autoionising Rydberg Electron Wavepacket Dynamics in NO V G Stavros, R A L Smith, J R R Verlet and H H Fielding, Kings College, London, UK

Molecular Photoionisation: High Resolution and Time Dependence Ch Jungen, Universit de Paris-Sud, Orsay, France

Oriented Molecule Photoelectron Angular Distributions of  $CF_4$  P Downie and I Powis, University of Nottingham, UK

Photoelectron-fragment Ion Correlations and Fixed-molecule Angular Distributions from Velocity Imaging Coincidences J H D Eland, M Takahashi and Y Hikosaka, University of Oxford, UK

Dissociation Dynamics Studied Using (1+1) REMPI-PES via a Fast Predissociative State of Ammonia Jijun Xu, Guohui Li, Guohe Sha, Bo Jiang, Cunhao Zhang and Jinchun Xie, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

Pulsed Field Ionization - Photoelectron Photoion Coincidence Spectroscopy with Synchrotron Radiation: The Heat of Formation of the  $C_2H_5^+$  Ion Tomas Baer, University of North Carolina, Chapel Hill, USA, Y.Song, C.Y. Ng, Iowa State University, Ames, USA, Jianbo Liu, Wenwu Chen, Lawrence Berkeley National Laboratory, Berkeley, USA

Transition State Dynamics of the OH + H<sub>2</sub>O Hydrogen Exchange Reaction Studied by Dissociative Photodetachment of H<sub>3</sub>O<sub>2</sub>- H-J Deyerl A K Luong, T G Clements and R E Continetti, University of California San Diego, La Jolla, USA

Mass Selective Gas Phase Study of ClO, OClO, ClOO and ClAr by Anion-ZEKE-Photoelectron Spectroscopy V Distelrath and U Boesl, Technische Universitt Mnchen, Garching, Germany

The Stability of High Rydberg States in the Presence of Time-dependent Inhomogeneous Fields T P Softley, S R Procter and M J Webb, University of Oxford, UK

PFI-ZEKE Photoelectron Spectra of the Methane Cation and the Dynamic Jahn-Teller Effect R Signorell and F Merkt, ETH Zurich, Switzerland

Pulsed Field Ionisation ZEKE Spectroscopy of Cresols and their Aqueous Complex Internal Rotation of Methyl Group and Intermolecular Vibrations M Fujii, Institute of Molecular Sciences, Okazaki, Japan

Resolved High Rydberg Spectroscopy of Polyatomic Molecules and Van der Waals Clusters K Siglow and H J Neusser, Technische Universitt Mnchen, Garching, Germany

Stabilization of Molecular Atoms T. Uzer, Georgia Institute of Technology, Atlanta, USA, E Lee and D Farrelly, Utah State University, Logan, USA

Threshold Ion-Pair Production Spectroscopy (TIPPS) of H<sub>2</sub> and D<sub>2</sub> R C Shiell, X K Hu, Q Hu, and J W Hepburn, University of Waterloo, Waterloo, Canada

Field Induced Ion-pair Formation from ICI Studied by Optical Triple Resonance S Wang, K P Lawley, T Ridley and R J Donovan, University of Edinburgh, UK

Ion-pair Formation Observed in a Pulsed-field Ionisation Photoelectron Spectroscopic Study of HF A J Yenchu, State University of New York, Albany, USA, M C A Lopes, Universidade Federal de Juiz de Fora, Brazil, G C King University of Manchester, UK, M Hochlaf, Universit de Marne-la-Vallee, France, Y Song and C K Ng, Iowa State University, Ames, USA

Recombination of Simple Molecular Ions Studied in Storage Ring M Larsson, Stockholm University, Sweden

Resonance-enhanced Multiphoton Ionisation Photoelectron Spectroscopy of the ClO Radical: the C<sub>2</sub>S- state  
D H A ter Steege, M Smits, C A de Lange, University of Amsterdam, The Netherlands, N P C Westwood,  
University of Guelph, Canada, J B Peel, La Trobe University, Bundoora, Australia, L Visscher, Vrije  
Universiteit, Amsterdam, The Netherlands

Spectroscopy of Excited Electronic States of Carbon Anions above the Detachment Threshold F Gthe, M  
Tulej, M Pachkov and J P Maier, Universitt Basel, Switzerland

Spectroscopic Observations of Vibrationally Mediated Slow Electron Capture M A Johnson and C E H  
Dessent, Yale University, New Haven, USA and The University of York, UK

Charge Localization and Charge Delocalization Investigated by Multiphoton Ionization High-resolution  
Photoelectron Spectroscopy R Weinkauff, Heinrich Heine Universitt, Dsseldorf, Germany

Concluding Remarks J Jortner, Tel Aviv University, Israel

### **5. 18th International Meeting of the Molecular Graphics and Modelling Society.**

Modelling Biomolecular Mechanism: From States to Processes at the Atomic Level April 5-8, 2000 at the  
University of York, UK

The meeting addresses the modelling of Biomolecular mechanisms and includes contributions leading  
computational scientists and experimentalists. In biomolecular systems, one often cannot simulate  
ensembles, but concentrates on single molecules. The size, complexity and spatial and temporal  
heterogeneity of biomolecular processes makes them extremely challenging. Of particular note are  
presentations on "reaction path" computations, which include "static" and explicit dynamic considerations  
of long-time/improbable processes. The experimental work represents some time-resolved and  
single-molecule techniques. The computational work also includes combined QM/MM potentials for  
studying reactive processes.

April 5-8, 2000 at the University of York, UK

\* Further Details & Information

Meeting Web Site at <http://www.mgms.org/york2000> Information on the Scientific Programme,  
Contributions, Registration and Travel available on the Web site

\* Meeting Agenda

The meeting focuses on the study of biomolecular processes including chemical reactions, protein folding,  
transport & diffusion and energy transduction. The meeting showcases advances in theoretical and  
computational approaches to studying biomolecular processes as well as powerful single molecule and  
time-resolved experimental techniques. With contributions from leading international researchers, the  
meeting provides an important and timely opportunity to review and stimulate discussion across the many  
disciplines addressing the mechanistic aspects of structure-function relationships in biological processes at  
the atomic level.

\* Scientific Programme (see <http://www.mgms.org/york2000/programme.htm>)

Abstracts will be published in the Journal of Molecular Graphics and Modelling  
(<http://www.elsevier.nl/locate/jmngm>).

– Sessions Include:

Pathway Methods; Enzyme Reactions; Transport & Diffusion; Folding; Manipulation; Energy Transfer &  
Transduction; Solution Dynamics

– Confirmed Invited Speakers and Titles:

HJC Berendsen, Univ. of Groningen "Diffusion-limited enzyme catalysis: Lecithin into phospholipase A2"  
Bernie Brooks, NIH (Title TBA)

Charlie Brooks, TSRI "Protein Folding Landscapes, Mechanism and Kinetics: Insights from Theory and  
Simulation"

Leonor Cruzeiro-Hansson, Herriot-Watt Univ. "Vibrational energy transfer as the first step in protein  
function"

Ron Elber, Cornell "Long time dynamics of biomolecules using the stochastic path approach"

Stefan Fischer, Univ. of Heidelberg "Molecular kinematics: essential motion and energetics of slow (> 1us)  
processes in proteins."

Hans Frauenfelder, Los Alamos Natl Laboratory "Complexity in protein dynamics and protein reactions."  
 Hermann Gaub, Univ. of Munich (Title TBA; topic on AFM-related work)  
 Ian Hillier, Univ. of Manchester "What can QM/MM calculations tell us about enzyme reactions?"  
 Martin Karplus, Univ. of Strasbourg/Harvard "Free energy simulations in the new millennium"  
 Peter Kollman, UCSF "Molecular dynamics simulations on protein and nucleic acid systems: Entering the era of structure and free energy"  
 Andy McCammon, UCSD "Dynamics of Molecular Recognition"  
 Justin Molloy, Univ. of York "Use of optical techniques to probe the mechanism of energy transduction of single molecular motors"  
 David Perahia, CNRS Orsay "Study of conformational pathways in proteins: methods and applications"  
 Simon Phillips, Univ. of Leeds "Towards a movie of catalysis in copper amine oxidases"  
 Rudolf Rigler, Karolinska Institute "Spectroscopy of Single Biomolecules: The fluctuating enzyme"  
 Benoit Roux, Univ. of Montreal "Simulating the Flow of Ions across Membrane Channels"  
 Klaus Schulten, Univ. of Illinois "Steered Molecular Dynamics to Study Biopolymer Association and Stretching"  
 Lorna Smith, Univ. of Oxford "Characterisation of denatured and partially folded protein conformations"  
 John Straub, Boston Univ. "Direct computation of long time processes in peptides and proteins"  
 Michael Schaefer, Univ. of Strasbourg "Structural and thermodynamic characterization of polypeptides by computer simulation: Helices, beta-hairpins, and chameleons."  
 Wilfred van Gunsteren, ETH Zurich "Computer simulation of the reversible folding of peptides"  
 RJP Williams, Univ of Oxford "Coupling between electron and proton energies in Proteins"  
 Peter Wolynes, Univ. of Illinois "Pure and Applied Protein Folding Kinetics."  
<http://www.mgms.org/york2000>

## **6. MOLECULAR and IONIC CLUSTERS CONFERENCE - 2000**

Toulouse, France, April 16-21 2000

This conference follows a series of very successful Gordon conferences, with the last two held at Il Ciocco, Italy (1996) and Ventura, California (1998). The conferences have taken place biannually, alternating between the US and Europe. This alternation underlines the international aspect of the field and provides a regular channel for exchange between scientists in North America and Europe. The year 2000 conference will not be a Gordon conference, since the Gordon Research Conferences do not have an official site in France. However, it will adhere to the Gordon Conference format, and be followed by a GRC planned for 2002 back in Ventura. There will be room for 120-130 participants.

Conference topics will include molecular and ionic clusters ranging from small to large sizes, from both experimental and theoretical perspectives. Leaders in the field will discuss areas such as spectroscopy, structure, dynamics, thermodynamics, etc... for both neutral and ionic complexes. Thanks to the success of the preceding conferences, this series has become one of the premier meetings on clusters of all types. The conference will take place at the Congress Center in Toulouse. Accommodations will be at the in-site Mercure hotel.

Current sponsors include: The European Community (TMR and INCO programs), CNRS. Organizers:

Philippe BRECHIGNAC & Nadine HALBERSTADT

Philippe.Brechignac@ppm.u-psud.fr & nhalbers@irsamc1.ups-tlse.fr

Labo. Photophysique Moleculaire

Labo. Physique Quantique, IRSAMC

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Here is the address for the web site: <http://www.irsamc.ups-tlse.fr/irsamc/mic2000.htm>

## **7. DYNAM 2000: Satellite Meeting of the Xth ICQC on Chemical Dynamics**

Arcachon, France, 31 May - 3 June 2000 (just before the International Conference on Quantum Chemistry, Xth ICQC, in Menton)

This meeting will cover the theoretical aspects of Classical, Semi-Classical and Quantum Molecular Dynamics which are relevant to Chemistry. The topics will therefore include theoretical and computational developments, as well as applications to specific systems in gas phase and condensed media.

Organizer: J.C. Rayez, Laboratoire de Physico-Chimie Moléculaire, Université Bordeaux - 33405 Talence (F)

Tel: +33 (0)5 56 84 66 08 - Fax: +33 (0)5 56 84 66 45 e-mail: rayez@cribx1.u-bordeaux.fr

Co-organizers: J.A. Beswick IRSAMC Université Paul Sabatier - 31062 Toulouse (F) Tel: +33 (05) 61 55 60 09 - Fax: +33 (0)5 61 55 60 6 e-mail: beswick@irsamc1.ups-tlse.fr

C. Leforestier LSDSMS - Université du Languedoc - 34095 Montpellier (F) Tel: +33 (0)4 67 14 33 39 - Fax: +33 (0)4 67 14 48 39 e-mail: lefores@lsd.univ-montp2.fr

Invited speakers having already accepted: F. Aguillon (Orsay), A. Bastida (Murcia), S. Cavalli (Perugia), D. Clary (London), H. Dieter-Meyer (Heidelberg), R. Kosloff (Jerusalem), D. Manolopoulos (Oxford), C. Meier (Toulouse), G. Parlant (Montpellier), O. Roncero (Madrid), R. Schinke (Göttingen), S. Smith (Brisbane), A. Varandas (Coimbra), J.Zhang (New-York).

Students and Postdocs wishing to participate in the meeting and to present a poster may apply for financial aid. The amount of support will depend on our success for attracting external fundings. Please send an abstract as soon as possible to: Philippe Halvick - Laboratoire de Physico-Chimie Moléculaire, Université Bordeaux, 33405 Talence Cedex (France) Tel: +33 (0)5 56 84 83 77 - Fax: +33 (0)5 56 84 66 45 e-mail: halvick@lpct.u-bordeaux.fr

For more information, check out our web site: <http://www.lpcm.u-bordeaux.fr/infos/dynam2000>

## **8. 55th OHIO STATE UNIVERSITY INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY**

June 12-16, 2000, Columbus, Ohio, USA

### **PLENARY SPEAKERS**

Jose Cernicharo, CSIC Madrid

Frederic Merkt, ETH Zurich

John Hepburn, University of Waterloo

David Nesbitt, JILA, University of Colorado

Gerard Meijer, University of Nijmegen

Timothy Steimle, Arizona State University

Martin Gruebele, University of Illinois, Coblentz Award Winner

### **SPECIAL SESSIONS**

Several special mini-symposia are planned for this year's meeting. Wolfgang Ernst, Penn State University, is organizing a session entitled, "Jahn-Teller/Renner-Teller" which will cover the classical Jahn-Teller and Renner-Teller effects as well as other vibronic interactions. Invited speakers will include Horst Koepfel, University of Heidelberg; Anthony Merer, University of British Columbia; and Timothy Barckholtz, JILA. A second mini-symposium is being organized by Michael Duncan, University of Georgia, on the subject of "Metal Complexes" from diatomics to moderately large clusters. Invited speakers for this mini-symposium include Paul Dagdigan, Johns Hopkins University, and Gert von Helden, University of Nijmegen. A third mini-symposium is being organized by John Maier, University of Basel, on "Negative Ions." The symposium will cover both experiments and theory involving negative ions. Invited speakers will include Carl Lineberger, University of Colorado; and Jack Simons, University of Utah. A session on theory is being organized by Russell Pitzer, Ohio State University, featuring a talk by Michael Robb, University College London.

### **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 (see overleaf) 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 will again 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 will again accept credit cards. You will be able to charge your entire pre-registration (conference and dorm) fee to your Visa or MasterCard credit card (see registration page). For those few not pre-registering, you will be able to charge your dorm accommodations upon check-in, AND your Symposium registration fee at the Smith Lab registration desk. 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. At this time we are working to implement on-line pre-registration. Whether this will be available for next June's meeting is not yet known. Please check the Symposium WWW site for progress.

#### INSTRUCTIONS FOR ABSTRACT SUBMISSION

The abstract book will be printed directly from a computer file this year. All abstracts whether submitted electronically or on paper should have the style indicated below for uniform appearance in the abstract book. This appearance will be automatically created for abstracts submitted electronically but of course must be created by the author for paper abstracts. Abstracts on paper will be scanned and reproduced at approximately a 1:1 scale.

The formatting details for contributed papers can be found in the paper version of this announcement which should be received by persons on the symposium mailing list in January 2000 or are viewable at our Web site. Briefly, paper abstracts will be scanned and must be smaller than 6.75 inches (17.1cm) wide and 4.25 inches (10.8cm) long. Note at the bottom paper category (see below) and time (5, 10, 15 min) requested for presentation.

#### IMPORTANT POINTS TO NOTE

1. If submitting by the traditional paper method, please send a total of three copies of each abstract, at least one of high quality for electronic reproduction.
2. Underline the name of the person presenting the paper.
3. Remember to indicate in the comment line if the speaker is to be considered for the Rao Prize (see below for complete instructions).
4. DEADLINE FOR RECEIPT OF ALL ABSTRACTS IS MARCH 1, 2000.
5. For the time of your presentation, check the program, available by April 15 on our WWW site.

#### SESSION CATEGORIES

1. Electronic (large molecules)
2. Electronic (small molecules)
3. Theory (quantum calculations)
4. Theory (other)
5. Infrared
6. Raman
7. Microwave
8. Jet and Beam Spectra
9. Radicals and Ions
10. Matrix
11. Condensed Phase
12. Mini-symposium: Jahn-Teller/Renner-Teller

13. Mini-symposium: Metal Complexes

14. Mini-symposium: Negative Ions\*

\*The Journal of Molecular Spectroscopy is planning to publish a review article based upon the invited talk of Carl Lineberger in this mini-symposium. If you will be writing a paper on the subject of the abstract that you submit to the symposium and wish it to be published in the same issue as the review article, it should be submitted to the journal by 1 Aug., 2000. All such articles will be reviewed.

#### ELECTRONIC ABSTRACT SUBMISSION (EAS)

To submit your abstract electronically, you must download the instructions. To accomplish this, do one of the following:

1. Access the Symposium World Wide Web site (URL– <http://molspect.mps.ohio-state.edu/symposium/>) and follow the menu to electronic abstract submission instructions, or
2. Anonymous logon to our FTP site, [molspect.mps.ohio-state.edu](http://molspect.mps.ohio-state.edu) and download the file [/symposium/submit](#), or
3. Send an email to [eas@molspect.mps.ohio-state.edu](mailto:eas@molspect.mps.ohio-state.edu). The email should contain only the subject line: EAS Instructions.

When you have completed your electronic abstract, just email it to our test address for viewing or to the above email address for actual submission. Upon receipt, your document will be processed by a LaTeX- 2e compiler and you will automatically receive an email reply indicating either a successful submission or a problem. If you submit electronically and you receive confirmation of a successful submission, you need do nothing more. Once you have successfully submitted your abstract, DO NOT resubmit it or a "revised" copy electronically. DO NOT send us an additional paper copy. Either action could result in your abstract being included twice in the program. Please note that we can only handle one format for electronic submission. LaTeX was chosen because of its support by several American professional societies and widespread use in the worldwide scientific community.

**SPONSORSHIP** We are pleased to announce our anticipated sponsorship for the 55th Symposium. We anticipate that principal funding will come from the Army Office of Research (ARO). We are most grateful to ARO for their support. We are also receiving support from The Ohio State University through the Chemistry and Physics Departments, and the College of Mathematical and Physical Sciences. Our anticipated Corporate sponsors are Coherent Inc. and General Valve. As in the past, Coherent will sponsor the coffee and doughnuts. The support of General Valve will allow us to reduce the cost of the picnic for students. Lambda Physik and Academic Press are our Contributing Sponsors. Academic Press will support a review lecture by Carl Lineberger in the mini- symposium on negative ions. At this time, Bruker, Laser Photonics and Newport Corp. have also confirmed their plans to exhibit at the Symposium. These and other sponsors will have exhibits at the Symposium and we encourage you to visit their displays. **RAO PRIZE** The three Rao Prizes for the most outstanding student talks at the 1999 meeting will be presented. The winners are R. Timothy Bonn, University of Pennsylvania; Sachiko Itono, Ochanomizu University; and Sabine F. Deppe, Universitat Gottingen. The Rao Prize was created by a group of spectroscopists who, as graduate students, benefitted from the emphasis on graduate student participation, which has been a unique characteristic of the Symposium. This coming June three more Rao Prizes will be awarded. In order to be eligible for the Rao Prize, a student must (i) be primary author of the work being presented; (ii) be the actual presenter of the talk; (iii) never have competed for the Rao Prize prior to this year; and (iv) not have completed a Ph.D. thesis prior to March 1, 2000. If a student wishes to compete for the Rao Prize, he or she should indicate this in the comment area of the abstract (due by March 1) for the talk they wish to be judged and send a letter from the research supervisor certifying that the student meets all four of the above requirements. The letter of certification is not a nomination letter and will not be considered by the prize judges. The award will be administered by a Prize Committee chaired by Arlan Mantz, Connecticut College, and comprised of Michael Heaven, Emory University; Angela R. Hight Walker, NIST; Kevin Lehmann, Princeton University; John Muentner, University of Rochester; and Deanne Snavely, Bowling Green State University. Any questions or suggestions about the Prize should be addressed to the Committee. Anyone (especially post-docs) willing to serve on a panel of judges should contact Arlan Mantz (e-mail: [awman@conncoll.edu](mailto:awman@conncoll.edu)).

**PICNIC** The Symposium picnic will be held on Wednesday evening, June 14, at the Fawcett Center. The cost of the picnic is included in your registration (at below cost to students), so that all may attend the event. The Coblenz Society is the host for refreshments at 6:30pm before the picnic at 7:45pm at the Fawcett Center.

**LIABILITY** The Symposium fees DO NOT include provisions for the insurance of participants against personal injuries, sickness, theft or property damage. Participants and companions are advised to take whatever insurance they consider necessary. Neither the Symposium executive committee, its sponsors, nor individual committee members assume any responsibility for loss, injury, sickness, or damages to persons or belongings, however caused.

**REGISTRATION**

Preregistration is highly encouraged with a special rate for those prepaying on or before May 15, 2000.

Registration Type Prepaying After May 15 (circle one)

Regular\* \$75 \$100

Student\* \$25 \$35

\*Please note that the registration fee includes the cost (students subsidized) of the picnic on Wednesday.

Tickets for accompanying persons may be purchased for \$25 each.

Give name as you wish it to appear on your name tag.

.....

Family Name First Name Middle (if you want it on name tag)

.....

Department/Division

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University/Organization (to appear on name tag) Street Address

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Make checks (U.S. currency only payable through a US bank) payable to: International Symposium on Molecular Spectroscopy

Send to: Terry A. Miller, International Symposium on Molecular Spectroscopy, The Ohio State University, 120 W. 18th Ave. Columbus, OH 43210

**DORMITORY RESERVATION**

The Ohio State Dormitories have a limited number of rooms. Preregister by May 15 to guarantee your space. The prepayment and regular dormitory rates as indicated below are per person per night.

Submitting an abstract does NOT preregister you.

(Indicate one) Prepayment Regular

(after May 15)

Single room \$38.00 \$43.00

Double room \$19.00 \$24.00

Graduate students, (dbl room) \$18.00 \$23.00

Please indicate which nights you require accommodations. (NOTE: Dorm will NOT open until 10:00am June 11)

Sunday, June 11 ..... If requesting double, indicate:

Monday, June 12 ..... male .... female ....

Tuesday, June 13 ..... or name of roommate.

Wednesday, June 14 ..... .....

Thursday, June 15 ..... Roommate Name

Friday, June 16 .....



## **9. ATOMS, MOLECULES AND QUANTUM DOTS IN LASER FIELDS: FUNDAMENTAL PROCESSES**

PISA, Italy, June 12-16, 2000

This is a Satellite conference to ICAP-2000 International Conference on Atomic Physics, Firenze, June 6-10, 2000.

The Conference is jointly organised by:

- Istituto di Chimica Quantistica ed Energetica Molecolare del CNR, Pisa;
- Istituto di Fisica Atomica e Molecolare del CNR, Pisa;
- Dipartimento di Chimica e Chimica Industriale dell' Universita' di Pisa;
- Dipartimento di Fisica dell'Universita' di Pisa;
- Scuola Normale Superiore, Pisa

Further information: <http://www.icqem.pi.cnr.it/rizzo/Pisa2000.html>

and Pisa2000 Conference, ICQEM-CNR - Via Risorgimento, 35, I-56126 PISA (Italy)

Tel.: +39 050 918240, Fax: +39 050 502270

E-mail: [pisa2000@indigo.icqem.pi.cnr.it](mailto:pisa2000@indigo.icqem.pi.cnr.it)

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phone: ++39-50-918240, fax: ++39-50-502270, E-Mail: [lami@indigo.icqem.pi.cnr.it](mailto:lami@indigo.icqem.pi.cnr.it) ,

<http://www.icqem.pi.cnr.it>

## **10. Atomic and Molecular Interaction (AMI) Gordon Conference.**

This year's AMI Gordon Conference will be held at Colby Sawyer College in New London, New Hampshire from July 2nd to July 7th. The meeting will include 29 invited talks (Speaker list is below) on both experimental and theoretical subjects associated with the conference title. Subjects to be covered at this year's meeting include; non-adiabatic processes, bimolecular and unimolecular reactions, surface/molecule interactions, chemistry in clusters, low-temperature chemistry and intra and inter molecular energy transfer. In addition there will be two poster sessions. All attendees, especially graduate students and postdocs, are encouraged to present a poster. Send poster abstracts to David W. Chandler at MS 9055, PO Box 969, Sandia National Laboratory, Livermore CA, 94551.

The Gordon Conference attendance will be limited to 120 participants including speakers. Those interested in attending please consult the Gordon Research Conference web pages:

<http://www.grc.uri.edu/> and <http://www.grc.uri.edu/programs/2000/atomic.htm>

To apply to attend the AMI-GRC, please fill out the email form at: [app@grcmail.grc.uri.edu](mailto:app@grcmail.grc.uri.edu) or by mail from: Conference Application Gordon Research Conferences University of Rhode Island P.O. Box 984 West Kingston, RI 02892-0984 USA 401-783-4011 401-783-7644 (FAX)

Invited Speakers List: Fred Temps (University Kiel, Germany) Ned Sibert (Univ. of Wisconsin, USA) Mike Ashfold (University of Bristol, England) Kopin Liu (IAMS, Taiwan) George Schatz (Northwestern University, USA) David Parker (Univ. of Nijmegen, the Netherlands) Steve Gray (Argonne National Laboratory, USA) David Nesbitt (Univ. of Colorado, USA) Michael Collins (Australian National University, Australia) Piero Cassavechia (Univ. of Perugia, Italy) Carl Hayden (Sandia National Laboratory, USA) Kirk Peterson (Pacific Northwest Laboratory, USA) Wei Kong (Oregon State University, USA) Antonio Lagana (University of Perugia, Italy) Jim Valentini (Columbia University, USA) Octavio Roncero (I.M.A.F.F. (C.S.I.C.), Spain) Curt Wittig (University of Southern California, USA) Greg Sitz (University of Texas, USA) Bret Jackson (University of Massachusetts-Amherst, USA) Arthur Utz (Tufts University, USA) Anthony Stone (Cambridge, England) Mike Pilling (Univ. of Leeds, England) Eric Herbst (Ohio State University, USA) Ian Smith (Univ. Birmingham, England) Charlie Parmenter (Indiana University, USA) Ad van der Avoird (Univ. of Nijmegen, the Netherlands) Steven Stolte (Free University of Amsterdam, The Netherlands) Jeremy Hutson (University of Durham, England) George Ewing (Indiana University, USA) Conference Chair: David W. Chandler, Sandia National Laboratory, PO Box 969, MS 9055, Livermore CA, 94551-0969, [chandler@ca.sandia.gov](mailto:chandler@ca.sandia.gov), FAX: 925-294-2276

Vice Chair: Albert F. Wagner, Argonne National Laboratory, Argonne IL, 60439,  
wagner@anchim.chm.anl.gov

### **11. 16TH INTERNATIONAL SYMPOSIUM ON GAS KINETICS**

JULY 23rd-27th, 2000 in CAMBRIDGE, U.K.

The 16th International Symposium of Gas Kinetics (gk2k), organised by the Royal Society of Chemistry Gas Kinetics Discussion Group will take place: JULY 23rd-27th, 2000 in CAMBRIDGE, U.K.

The meeting will be held in the Chemistry Department, Cambridge University, and participants will be accommodated in Robinson College, Cambridge.

The scientific programme will include sessions on:

Dynamics and Kinetics of Elementary Reactions

Atmospheric Chemistry

Combustion and Dynamics

Inter- and Intra- Molecular Energy Transfer

Chemistry in Extreme Environments

Plenary Lectures will be given by D.J. Nesbitt, M. Brouard, J.N. Crowley, C.E. Kolb, C.T. Bowman, P.J.

Dagdigian, R.E. Miller and P. Andresen. The Polanyi Lecture will be presented by J. Wolfrum and is entitled: "Laser Studies of the Kinetics of Homogeneous and Heterogeneous Processes: From Diatomics to DNA"

We strongly encourage you attend the symposium and to submit abstracts for scientific contributions. To register, please fill in and return the form at:

<http://www.gk2k.ch.cam.ac.uk/>

Completed forms may be submitted by email to: [gk2k@atm.ch.cam.ac.uk](mailto:gk2k@atm.ch.cam.ac.uk)

Alternatively forms may be posted to:

Gillian Southwell, 16th International Symposium on Gas Kinetics, University Chemical Laboratory,  
Lensfield Road, Cambridge, CB2 1EW, U.K. (FAX +44 1223 336362). Registrations should be returned by:  
FRIDAY JANUARY 7TH 2000

A full social programme is also planned, including tours of the Cambridge Colleges, a recital in King's College Chapel and a banquet in Robinson College Cambridge, where participants will be accommodated. Dr David Husain has kindly agreed to give the post-banquet speech.

A second circular with full details will be sent to all those expressing an interest in Spring 2000.

Further details will be made available on the gk2k website. Other enquiries should be made to the gk2k committee via email to [gk2k@atm.ch.cam.ac.uk](mailto:gk2k@atm.ch.cam.ac.uk).

The end of the gas kinetics symposium coincides with twenty-eighth international symposium on combustion, which will take place in Edinburgh, U.K. from 30/7/00 - 4/8/00. Details of that meeting are posted at

<http://www.efm.leeds.ac.uk/edin2000/>

The gk2k local organising committee. (Dr.R.A. Cox, Dr. D. Husain, Dr. D.M. Rowley and Dr. S.M. Ball)

### **12. MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS GORDON RESEARCH CONFERENCE**

Colby Sawyer College, New London, New Hampshire July 30 - August 4, 2000 The scientific program will include 22 invited 40 minute talks arranged into the following sessions: Herzberg Session, From Atom-in-Molecule to Supercritical Fluids, Imaging and Control, Quantum Dots, A Little of This and A Little of That, Light Harvesting Antenna Systems, and Time vs. Frequency Domains. In addition there will be four poster sessions. All attendees, especially graduate students and postdocs, are encouraged to present a poster. Grant applications are pending which would provide partial support (Conference Fee and travel) for early-career scientists who plan to present a poster. The Invited Speakers include: Ch. Jungen, F. Merkt, R. Lipson, W. Ketterle, A. Vilesov, T. Momose, J. Brennecke, C. Hayden, C. Blondel, P. Bucksbaum, S. Leone, J. Cao, U. Banin, M. Moskovits, P. McEuen, H.F. Davis, M. Gruebele, R. Van Grondelle, K. Schulten, S. Volker and D. Jonas.

To apply to attend, the MES&D - GRC, please fill out the form obtainable by email at:

app@grcmail.grc.uri.edu

or request a form from Conference Application

Gordon Research Conferences, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892-0984  
USA

401-783-4011, 401-783-7644 (FAX)

<http://www.grc.uri.edu/programs/2000/molspec.htm>

Conference Chair: Robert W. Field, Room 6-219, MIT, 77 Mass. Ave., Cambridge, MA 02139 (617)  
253-1489 (VOX), (617)-253-7030 (FAX), [rwfield@mit.edu](mailto:rwfield@mit.edu)

Vice Chairs: Elliot Bernstein, Department of Chemistry, Colorado State University, Fort Collins, CO  
80523-1872 (970) 491-6347 (VOX) (970) 491-1801 (FAX) [erb@lamar.colostate.edu](mailto:erb@lamar.colostate.edu)

James Skinner, Department of Chemistry, University of Wisconsin, Madison, WI 53706-1396 (608)  
262-0481 (VOX) (608) 262-9918 (FAX) [skinner@chem.wisc.edu](mailto:skinner@chem.wisc.edu)

### **13. ATOMIC AND MOLECULAR DATA FOR ASTROPHYSICS NEW DEVELOPMENTS, CASE STUDIES AND FUTURE NEEDS. JOINT DISCUSSION**

JD 1, August, 9-11, 2000 at the XXIVth GENERAL ASSEMBLY of the INTERNATIONAL  
ASTRONOMICAL UNION MANCHESTER, AUG. 7-18, 2000

Organized by IAU Commission 14: Atomic and Molecular Data Co-supporting Commissions: 15 (Physical Study of Comets, Minor Planets and Meteorites), 16 (Physical Study of Planets and Satellites), 29 (Stellar Spectra), 34 (Interstellar Matter), 36 (Theory of Stellar Atmospheres), 40 (Radio Astronomy), 44 (Space and High Energy Astrophysics).

#### **MOTIVATIONS**

The past few years have seen tremendous advances in observational techniques, both in space and on the ground. In the near future, several new ambitious and expensive spaceborne and ground based instruments will become available and provide a wealth of high quality observations in an extended range of wavelengths. The reduction, analysis and interpretation of the observational results requires, at each stage, increasingly extensive sets of atomic and molecular data especially since the objects studied are often in extreme physical conditions which cannot be reproduced in the laboratory and can be studied only by modelling. In this respect, it is the function of Commission 14 of the IAU to help keep the astronomers informed of the available data and of the programs undertaken in other communities, to favour the exchange of information in order to make the Atomic and Molecular Physics community aware of the needs of Astronomy for new data and, finally, to inform the program agencies of the needs for specific studies and funding in these areas. To this end, Commission 14 organizes a Joint Discussion at the next General Assembly of the IAU. The program is organized around topics corresponding to future or recent space missions or selected because they are fast moving and particularly in need of new laboratory data. In addition, case studies are included in which a particular species or process is analyzed from several angles in order to highlight its contribution to the interpretation of different astronomical observations or models. It is comprised of invited oral presentations and contributed posters.

Oral presentations and poster abstracts will be published in the proceedings to appear in:

Highlights of Astronomy (Vol. 12), 2000, J. Andersen Ed., PASP (San Francisco)

#### **SCIENTIFIC ORGANIZING COMMITTEE:**

S.K. ATREYA (USA), K.A. BERRINGTON (UK), J. CERNICARO (Spain),

TH. HENNING (Germany), S. JOHANSSON (Sweden), T. MILLAR (UK),

F. ROSTAS (France, Chairperson), S. SAITO (Japan), D. SCHULTZ (USA),

P.SMITH (USA, Co-Chairperson), W.- L. TCHANG-BRILLET (France, Editor),

E. VAN DISHOECK (Netherlands)

#### **CONTACT ADDRESS:**

Francois ROSTAS, Observatoire de Paris-Meudon, 92195 Meudon Cx, France.

Telephone: +33 (0)1 45 07 75 65, Facsimile: +33 (0)1 45 07 71 00

e-mail: [Francois.Rostas@obspm.fr](mailto:Francois.Rostas@obspm.fr)

WEBSITE: <http://www.obspm.fr/IAU14/jd1.html>

VENUE, REGISTRATION, ABSTRACT SUBMISSION, TRAVEL GRANTS:

Please visit our website for details.

DEADLINES:

Peregistration: As soon as possible.

Application for travel grants: February 15, 2000.

Poster abstracts: February 15, in preliminary form, especially for grant applicants May 15 in final form for all participants.

Registration to the IAU General Assembly: Reduced rate: May 1, 2000.

SCIENTIFIC PROGRAM (as of January 28, 2000)

WEDNESDAY, AUGUST 9, MORNING

GRAINS

Grains in Astronomy:

Overview A. Witt (USA)

The Formation and Evolution of Interstellar Dust A. Jones (France)

Laboratory Analogues of Cosmic Dust H. Mutschke (Germany)

"GEMS" J. Bradley (USA)

INFRARED OBSERVATORIES (ISO / SOFIA / SIRTf / FIRST)

Introduction E. van Dishoeck (Netherlands)

Infrared Observations of Ices A. Boogert (USA)

PAHs T.B.A

Silicates R. Waters (Netherlands)

Gas-phase Atomic and Molecular Species J. Lacy (USA)

THURSDAY, AUGUST 10, AFTERNOON POSTER SESSION

FRIDAY, AUGUST 11, MORNING GAS-SURFACE REACTIONS

Surface Reactions in Interstellar Space E. Herbst (USA)

Theoretical Simulations J. Takahashi (Japan)

Grain Surface Chemistry and Solid State Photochemistry W. Schutte (Netherlands)

H<sub>2</sub> IN SPACE D.R. Flower(UK)

THE WATER MOLECULE

H<sub>2</sub>O in Young Stellar Objects T.B.A.

H<sub>2</sub>O in the Sun and Stars P. Bernath (Canada)

H<sub>2</sub>O in Comets, Observations and Models J. Crovisier (France)

ASTRONOMY, PHYSICS AND CHEMISTRY OF H<sub>3</sub><sup>+</sup> T. Oka (USA)

FRIDAY, AUGUST 11, AFTERNOON

THE FUSE SPACE MISSION,

Atomic and Molecular Data, Needs and Availability K. Sembach (USA)

THE CHANDRA, ASTRO-E AND XMM SPACE MISSIONS,

Atomic Data for X-ray Astronomy N. Brickhouse (USA)

THE FERRUM PROJECT

New Experimental f-values for FeII S.Johansson (Sweden)

SOLAR SYSTEM MISSIONS

Laboratory Data for Exobiologically Oriented

Studies of Titan F. Raulin (France)

Laboratory Chemical Kinetics and Outer Planets R. Kaiser (China, R)

IR spectroscopy and Jupiter P. Drossart (France)

Clouds and Chemistry of Jupiter's Atmosphere S. Atreya (USA)

Atmospheric Probes T. Owen (USA)

POSTER CONTRIBUTIONS

Poster contributions by all participants are heartily encouraged as useful complements to the oral presentations. In particular, information and demonstrations concerning data bases are welcome.

It is planned to publish the poster abstracts in the proceedings of the Joint Discussion which will appear in Highlights of Astronomy (Vol. 12).

Preliminary abstracts should be submitted before February 15, 2000.

Final abstracts in LaTeX form must be received before May 15, 2000

For details, please visit our website: <http://www.obspm.fr/IAU14/jd1.html>

#### **14. THE BRIJUNI CONFERENCE BRIJUNI (BRIONI) ISLAND, CROATIA**

28.August-1.September 2000 Important problems for the XXI century

Important problems that confront science in future will be reviewed at the THE BRIJUNI CONFERENCE.

The scope is limited to some areas of science, and omission of very important other issues does not mean ignorance but rather limited time available. The issues that will be reviewed are: its structure and how to explore it. Fundamental properties of matter and materials is there room for radically new ideas where do we come from and where do we go to? At the conference the discussion periods are assigned significant lengths of time and the oral presentations are designed to form a framework for meaningful discussion. Apart from the usual aim of developing an up-to-date perspective of the present state of a given topic, the fundamental scientific philosophy behind the series of conferences is the stimulation of cross-disciplinary flow of knowledge and expertise from both the experimental and theoretical standpoints.

General information: Apart from the invited presentations there will be both oral and poster contributions; however the number of oral presentations will necessarily be limited. The registration fee is \$180 (\$60 students). For more details and the updated information see:

<http://www.brijuni-conference.irb.hr>

Deadlines: The conference attendance is limited to 80 participants (excluding accompanying guests). As a consequence it is important that, if you wish to participate, you should return the form below as soon as possible, preferably by 1 May 2000 and certainly no later than 1 Jun 2000 when the final reservations at the Brioni Conference Centre must be confirmed. Please indicate below how certain you are of coming in the event that the conference is oversubscribed.

Application should be sent by email to: [dbosanac@faust.irb.hr](mailto:dbosanac@faust.irb.hr)

or alternatively to the address:

S. Danko Bosanac, Institut Rugjer Boskovic, 10001 Zagreb, Croatia

Tel: +385 1 4561 038, Fax: +385 1 4680 245

#### **BRIJUNI CONFERENCE APPLICATION FORM**

NAME (including accompanying person/s)

.....  
.....

ADDRESS (including email)

.....  
.....  
.....

TITLE OF CONTRIBUTION

.....  
.....

#### **15. Faraday Discussion 117 - EXCITED STATES AT SURFACES**

The University of Nottingham, UK, 4-6 September 2000

Many interfacial processes implicitly involve the creation and decay of excited states. This Discussion will highlight their role in experimental and theoretical surface science. We shall consider a wide range of phenomena including surface spectroscopies and reactions to arrive at a deeper understanding of the main issues by explicitly including a description of transient states.

Excited electronic states play a pivotal role in measurements in both the energy and time domain. Hole decay in optical spectroscopies has a long history but the advent of newer probes (e.g. multiphoton photoelectron emission) with improved resolution suggests that we are now in a position to test some of the long-standing

paradigms. Many interesting resonance phenomena have been observed in electron energy loss spectroscopy from adsorbates and again new theoretical descriptions are required. The explosion of interest in scanning probe microscopies has focussed attention on the behaviour of processes in real space. The injection of electrons into molecular states at low energies gives rise to diffusion and complex restructuring in adsorbate layers. Elementary models have been proposed within the framework of Frank-Condon dynamics but with the emergence of high quality (albeit ground-state) electronic structure calculations is it possible to formulate excited state scenarios? The Discussion will also focuss on excited molecular states interacting with surfaces. The dynamics of a state-prepared molecule when it nears a surface is amazingly complicated with a wide range of final states possible (dissociation, scattering etc.). The interaction with the surface atomic and electronic degrees of freedom gives rise to transient excited states that dissipate energy and information. Are we yet in a position to arrive at a consistent theoretical description capable of including these effects? Experimental and theoretical contributions relating to the above areas or to any other, unmentioned, aspects of excited states at surfaces will be most welcome.

Papers should be concerned with NEW, UNPUBLISHED WORK and contributions of both an experimental and theoretical nature are welcome. Titles and abstracts, of about 300 words should be submitted no later than FRIDAY 3 SEPTEMBER 1999 to Professor S Holloway, Surface Science Research Centre, University of Liverpool, Liverpool, L69 3BX, United Kingdom; Fax: +44 (0) 151 708 0662; email: faraday@ssci.liv.ac.uk

#### ORGANISING COMMITTEE

Professor S. Holloway (Chair), Dr. G. R. Darling, Dr. R. G. Jones, Dr. D. Lennon, Professor E. Hasselbrink, Dr. K. Kolasinski, Dr. M. R. S. McCoustra.

The URL of the Faraday Discussions Homepage: <http://www.rsc.org/lap/confs/faradischeme.htm>

### **16. European Summerschool in Quantum Chemistry (ESQC-00)**

Riolo Terme, Italy September 17-30, 2000

The European summerschool in quantum chemistry (ESQC-00) will be arranged for the seventh time in September 2000. This 'extra' summer school will be arranged in Italy as a collaboration between the Universities of Bologna and Lund (ESQC is normally arranged every odd year in Sweden. The next 'ordinary' school will be arranged in 2001). The school is open to students from all over the world, but some priority will be given to participants from the southern and eastern parts of Europe. A number of scholarships will be available to support students who have difficulties in financing their participation. The total number of participants is limited to 70 and the organizers will make the final selection of students in case there are more applicants. ESQC-00 will be arranged at the same level as earlier summer schools and with the same schedule. The only difference is the location.

The school will be arranged in the village Riolo Terme, located in Romagna on the eastern slopes of the Appenines between Bologna and Rimini.

The deadline for the preliminary registration is Jan 31, 2000.

#### Organizing Committee

Professor Gian Luigi Bendazzoli (University of Bologna), Doctor Laura Gagliardi (Local Organizer, University of Bologna), Professor Paolo Palmieri (University of Bologna), President Gino Pasotti (IPS-International Products & Services, Milano and Terme di Riolo Bagni S.p.a., Riolo Terme, Italy), Professor Bjrn O. Roos (School Director, Lund University)

The URL of the ESQC-00 Homepage: <http://www.teokem.lu.se/esqc/00>

### **17. MOLEC 2000 (THE XIIIth MOLEC)**

Jerusalem, Israel, September 17 - 22, 2000

Steering Committee: V. Aquilanti, M. Ashfold, M. Baer, K. Bergmann, G.D. Billing, G. Delgado-Barrio, F. Gianturco, Z. Herman, R. McCarroll, V. Sidis, J.P. Simons, S. Stolte, J.P. Toennies.

Local Organizing Committee: Michael Baer (Chair), Y. Band, R. Kosloff, A. Lifshitz, N. Moiseyev, A. Nitzan, E. Pollak, S. Rosenwaks, A. Wilson-Gordon, D. Zajfman.

General Information: MOLEC 2000 will be held in Jerusalem starting September 17 and ending September

22, 2000. The venue is the 4-star hotel of Kibbutz Ramat Rachel, on the Jerusalem municipal border. The Meeting, the XIIIth in the series of MOLEC conferences, will follow in format the former conferences. Registration will be on Sunday, September 17 starting in the afternoon. There will be two morning sessions and two afternoon sessions on the Monday, Tuesday and Thursday. Wednesday afternoon will be free, for the excursion-tour (in Jerusalem). The Farewell dinner will be held Thursday night. Friday will be a half-day and the Meeting will end after lunch. All sessions will be plenary sessions. There will be three Poster sessions. Invited speakers (confirmed so far): L.H. Andersen, V. Aquilante, M. Barat, S. Berry, G.D. Billing, M.S. Child, L.S. Cederbaum, P. Crutzen, A. Dalgarno, G. Delgado-Barrio, A. Gonzales-Urena, G. Hancock, S. Haroche, Z. Hennis, J. Jortner, Y.T. Lee, C. Leforestier, R.D. Levine, C. Lifshitz, N. Makri, H.-D. Meyer, W.H. Miller, H. Nakamura, C.Y. Ng, B.J. Orr, M. Parrinello, U. Peskin, A.J.C. Varandas, and D. Yarkony. Progressive Registration Fee Deadlines: Normal rate: Up to 31/03/00: US \$200; up to 31/05/00: US \$250; after 01/06/00: US \$300. Student rate: Up to 31/03/00: US \$125; up to 31/05/00: US \$150; after 01/06/00: US \$175. Accompanying person: US \$50

Call for papers The topics covered by the conference include Reactive molecular collisions, Atmospheric chemistry, Astro-chemistry, Laser chemistry, Collisional energy exchange, Ion-molecule interactions, Electronic nonadiabatic effects and transitions, Collisions with surfaces and adsorbed species, Cluster studies, Photodissociation dynamics, Photodissociation and desorption at surfaces, Control of chemical processes, Doubly charged negative ions, Reactions in solution, Plasma, Ultra-cold atomic and molecular collisions, Resonance phenomena in molecular systems, Dissociative collisions, Unimolecular reactions, Molecular dynamics in dissipative systems.

The submission of abstracts is encouraged. Some contributions may be selected for oral presentation. Deadline for abstracts: July 15, 2000.

A Last Announcement has been circulated, with registration form and hotel reservation form. Should you wish to receive the Announcement or if you want to inquire about the meeting please contact Michael Baer (mmaer@netvision.net.il).

You are invited to visit the Conference website: <http://www.fh.huji.ac.il/~roib/MOLEC/index.htm> The Registration Form and the Form for Hotel Accommodations bookings may be downloaded from that site.

### **18. Chemistry and the Internet - ChemInt2000**

This note is to announce that web Abstract Submission form is now operational for the Chemistry and the Internet (ChemInt2000) meeting being held in at Georgetown University in Washington DC on September 23-26, 2000.

The draft program of invited speakers, workshops, markup language tutorial, and panel sessions is available on the meeting web site:

<http://www.chemint.org>

You are urged to look at the program and to consider submitting a poster paper to the meeting. Some 8-10 of poster papers will be selected for oral presentation at the meeting.

The main lecturers for the meeting will be:

Rene DePlanque, FIZ - Berlin; Jim Myers, Pacific Northwest Labs; Glen Hopkinson, Synopsys Scientific Systems; Jim Ostell, NIH/NLM/NCBI; Engelbert Zass, ETH; Henry Rzepa, Imperial College, London; Peter Murray-Rust, Nottingham University

The (current) corporate sponsors for the meeting are: SciVision, Internet Journal of Chemistry

Technical Sponsors are: ACS CINF Division, ACS COMP Division, The Chemical Structure Association (CSA), Georgetown University - Department of Chemistry, Special Libraries Association (SLA) Chemistry Division, Royal Society of Chemistry (RSC)

### **19. Stereodynamics of Chemical Reactions**

December 1 to 5, 2000

El Escorial (Madrid). SPAIN

Second Announcement

Format and Scope

This conference follows in scope and format the former meetings on Stereodynamics held in Jerusalem (1986), Bad Honnef (1988), Santa Cruz (1990), Assisi (1992), Gif sur Yvette (1994) and Bielefeld (1996). The programme comprises invited lectures, posters and oral presentations in a spacious surrounding with ample time for discussion. The conference covers the field of reactive and non-reactive collisions involving atoms, molecules and surfaces of solids and liquids as well as half collisions. Major topics to be addressed are:

- \* Stereocontrol of reactive collisions in the gas phase, on surfaces and in liquids.
- \* Orientation effects in beam-surface reactions.
- \* Brute force oriented molecules: collisions, spectroscopy, theory.
- \* Effect of molecular orientation and alignment in non-reactive collisions.
- \* Stereodynamics of photo-initiated reactions in Van der Waals complexes.
- \* Collisions of orbitally aligned atoms.
- \* In-situ measurements of orientation and alignment.
- \* New Techniques.

#### General Information

#### Programme

Arrival is at 1st of December, departure at 5th of December. The scientific programme will consist of invited lectures (30 to 40 min in length), poster and oral presentations (20 min in length) of a few contributed papers. Social events will include a visit to the Monastery of El Escorial, a visit to the Prado Museum in Madrid, and the Conference Dinner.

#### Proceedings

The conference proceedings will be published in a special issue of a Scientific Journal. All manuscripts should represent new and unpublished work. The contributions will be reviewed in the normal manner. The abstracts of invited lectures and contributed papers will be collected in the book of abstracts. Copies of it will be distributed to the participants.

#### Registration fee

The Registration fee is 60.000 pts., including conference kit, full board, visit to the Prado Museum, visit to the Monastery and Conference Dinner. Registration fee may be paid from August, 2000 on, to the following account:

Branch: Caja de Madrid 2038 1735 91

Account N: 6000402693

Please send a copy of the bank transfer to:

Dr. Stefan Skowronek, Instituto Pluridisciplinar, Universidad Complutense of Madrid, Juan XXIII, 1. 28040 Madrid

Conference fellowships are available upon request from Prof. A. Gonzalez Urea

#### Important Dates

\* Payment and Registration 31st of August 2000

\* Call for papers including further information and a list of invited speakers 30th of June 2000

#### Scientific Committee

R. Anderson (USA), V. Aquilanti (I), A. Gonzalez Urea (E), R.D. Levine (IL), H.J. Loesch (D), D. Parker (NL), J. Simons (UK), B. Soep (F), S. Stolte (NL), R. Vetter (F)

#### Local organisation

Angel Gonzalez Urea,

E-mail: stereody@eucmos.sim.ucm.es

Stefan Skowronek: Secretary of the Organising Committee.

Asuncin Garca Sousa: Secretary.

Address: Instituto Pluridisciplinar. Unidad de Lseres y Haces Moleculares. P Juan XXIII-1. 28040-Madrid. SPAIN.

Fax: ++34.91.394 3265

## 20. New Frontiers in Chemical Reaction Dynamics

"New Frontiers in Chemical Reaction Dynamics" will be held at the Pacificchem Meeting next December (December 14-19) in Hawaii. The organizers of this symposium are: Hiroki Nakamura, George Schatz, Kopin Liu, Robert Continetti, and Toshinori Suzuki.

This symposium has been organized to discuss the present status and the future prospects of chemical reaction dynamics with the participation of both the theorists and experimentalists. Rapid progress that has been made in the understanding of the triatomic model reactions will be reviewed, and the new research directions toward complex multidimensional systems will be highlighted in the discussion and presentations. The topics will include:

- (i) dynamical stereochemistry (orbital alignment, steric effect, and vector correlations),
- (ii) dynamics involving multiple potential energy surfaces (interference effects, non-adiabatic transitions),
- (iii) multidimensional dynamics (reactions of tetraatomic system or larger, calculations of cumulative reaction probabilities, statistical and non-statistical nature of the dynamics),
- (iv) imaging chemical dynamics (transition state spectroscopy, ultrafast spectroscopy, multiparticle coincidence)
- (v) laser-control of molecular processes (including intense field dynamics).

Invited speakers (confirmed so far) are:

Neumark, Leone, Suits, Houston, Haydon, Miller, Truhlar, Skodje, Yarkony, Albert, Seideman, Lee, Yang, Mebel, Park, Smith, Kasai, Matsumi, Nagata, Kondow, Takatsuka, Aoyagi, and Takayanagi.

We welcome contributed presentations. Details of the meeting can be found at the ACS web page ([www.acs.org](http://www.acs.org)) and in publications of the cosponsoring organizations in Japan, Canada, Taiwan, Australia, Korea.

George C. Schatz, Department of Chemistry, Northwestern University, Evanston, IL 60208-3113  
(847)491-5657, (847)491-7713 (fax) [schatz@chem.nwu.edu](mailto:schatz@chem.nwu.edu)

## 21. Faraday Discussion No. 118: Cluster Dynamics

University of Durham, UK 18-20 April 2001

Studies of atomic and molecular clusters are one of the growth areas of modern chemical physics. The last few years have seen major advances in both experimental and theoretical methods, and it is now possible to prepare and characterize a wide range of finite-size systems.

Abstracts of papers containing new, unpublished work (not reviews) are invited for consideration by the Organising Committee. Summaries of about 300 words should be submitted no later than 31 March 2000 to Prof. Jeremy M Hutson, Department of Chemistry, University of Durham, Durham, DH1 3LE, UK (email [J.M.Hutson@durham.ac.uk](mailto:J.M.Hutson@durham.ac.uk))

The Discussion will be focussed on studies that deal specifically with dynamical processes in a cluster environment and the interactions that determine them. The term "dynamics" will be interpreted widely, to include spectroscopic studies that probe multiple minima on a potential energy surface. The committee particularly welcomes papers in the following areas:

Reactions of clusters, Reactions induced by clustering, Transition-state spectroscopy, Photodynamics of clusters, Caging effects in clusters, Tunnelling in clusters, Global potential energy surfaces

ORGANISING COMMITTEE:

Professor Jeremy M. Hutson (Chairman), Professor Ad van der Avoird, Professor David C. Clary, Professor Peter J. Knowles, Professor Klaus Mueller-Dethlefs, Professor Anthony J. Stace,  
World-Wide Web home page: <http://www.dur.ac.uk/~dch0www/Staff/jmh/>

## 22. 26th International Symposium on Free Radicals.

"La Cittadella", Assisi, Italy, September 2-7, 2001.

Chairman: Piergiorgio Casavecchia (Universit di Perugia). A Web-page will become available at the beginning of the summer 2000.

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universit di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: [piero@dyn.unipg.it](mailto:piero@dyn.unipg.it) (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

## Special announcements

### INVITATION TO SUBMIT A PAPER

Announcement of a series of special issues year 2000 of **Zeitschrift fuer Physikalische Chemie (International Journal of Research in Physical Chemistry and Chemical Physics**, founded in 1887 by W. Ostwald and J.H. van't Hoff) in honour of Juergen Troe

Juergen Troe will be celebrating his 60th birthday in August 2000. His work has profoundly influenced our field and he has been on the editorial board of Zeitschrift fuer Physikalische Chemie for many years.

Following a good academic tradition, the Editor-in-Chief, Prof. F. Hensel has suggested to dedicate a series of special issues of this journal in the year 2000 to Juergen Troe, starting with August 2000.

In order to avoid disappointment of authors by delayed publishing of special issues of this kind, we have as guest editors obtained rather favourable timing conditions. **THE DEADLINE FOR THE RECEIPT OF ARTICLES OF THE AUGUST ISSUE IS 31 MARCH 2000**, but we will make efforts to include even slightly delayed articles in this issue. Later articles will simply go into the following issues. Thus the journal can guarantee publishing of the August issue on time, irrespective of delayed authors. **THE FINAL DEADLINE FOR RECEIPT OF LATE ARTICLES IS 1 AUGUST 2000**. All accepted articles will be published in 2000 and we expect to receive high-calibre papers of great current interest due to this smooth publishing schedule, as would fit for the person to be honoured. We plan to provide Juergen Troe with a landmark publication in our field.

All papers will be refereed in the usual way and should be sent to one of the guest editors listed below, best the one with research interest closest to the paper you submit.

Prof. Dr. Horst Hippler, Lehrstuhl fuer Molekulare Physikalische Chemie, Institut fuer Physikalische Chemie, Universitaet Karlsruhe, Kaiserstr. 12, DE-76128 Karlsruhe, Germany  
email: horst.hippler@chemie.uni-karlsruhe.de, Fax: +49-721-608 6524

Professor Klaus Luther, Institut fuer Physikalische Chemie, Universitaet Goettingen, Tammannstr. 6, DE-37077 Goettingen, Germany

email: kluther@gwdg.de, Fax: +49-551-393 150

Professor Martin Quack, Laboratorium fuer Physikalische Chemie ETH Zurich Zentrum, CH-8092 Zurich, Switzerland

email: quack@ir.phys.chem.ethz.ch, Fax: +41-1-632 1021

Professor Joerg Schroeder, Institut fuer Physikalische Chemie, Universitaet Goettingen, Tammannstr. 6, DE-37077 Goettingen, Germany

email: jschroe2@gwdg.de, Fax: +49-551-393 127

The journal **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) will publish articles in the area of "PHOTODYNAMICS FROM ISOLATED MOLECULES TO CONDENSED PHASES", in connection with the Havana Conference by the same title.

Contributions in the form of regular papers should be handed in preferably at the Conference (February 13-19, 2000), but other related contributions can be considered (deadline 31 March 2000). Further information from:

Professor V. Aquilanti, Department of Chemistry, University of Perugia, I-06123 Perugia, Italy.  
e-mail: aquila@dyn.unipg.it

### BOOKS and SOFTWARE

#### MOLSCAT Web pages

NASI GISS, who host the Web pages for the MOLSCAT program, have recently done some spring-cleaning. As a result, the URL that I and several other people have been using for MOLSCAT has changed. The MOLSCAT pages (containing FORTRAN source code and documentation for version 14) are now at

<http://www.giss.nasa.gov/molscat/>

Please would anyone else who has links to MOLSCAT on their page update the link?

For those who don't know, MOLSCAT is a general-purpose molecular inelastic scattering program, by Jeremy M. Hutson and Sheldon Green, with capabilities for atom + linear rigid rotor, atom + vibrating diatom, atom + symmetric, asymmetric or spherical top, and linear rigid rotor + linear rigid rotor.

There is also a general-purpose interface for adding other "coupling cases", which has been used (inter alia) for open-shell atom + diatom, atom + open-shell diatom, etc.

MOLSCAT also calculates pressure broadening and shifting cross sections, and post-processors are available for (some) differential cross sections, transport/relaxation cross sections and scattering resonances.

### **FREE SOFTWARE RELEASE ANNOUNCEMENT, MultiWell, version 1.01**

Macintosh and Unix/Linux versions are currently available. This version includes minor bug fixes and clearly stated copyright information. If you down-loaded the first release (v 1.0), please discard it and download this version in its place. Up-dated versions will be posted periodically.

With minor revisions, the source code can be compiled on other platforms (e.g. Windows). Compressed files can be downloaded from the MultiWell web site.

MultiWell web site: <http://aoss.engin.umich.edu/multiwell/>

MultiWell calculates time-dependent concentrations, yields, vibrational distributions, and rate constants as functions of temperature and pressure for unimolecular reaction systems which consist of multiple stable species, multiple isomerization reaction channels interconnecting them, and multiple fragmentation channels from each stable species. The stochastic method is used to solve the resulting Master Equation. Users may supply unimolecular reaction rate constants ( $k(E)$ 's), sums of states and densities of states (for RRKM theory), or optionally use the Inverse Laplace Transform method. Users can select for weak collision effects different collision models for down-steps including exponential, biexponential, generalized exponential, etc., and user-defined functions. Thermal, chemical activation, or user-defined functions can be used for the initial energy distribution.

The code is intended to be relatively easy to use. It is designed so that very complicated and very simple unimolecular reaction systems can be handled via the data file: no restructuring of the code or recompiling is necessary to handle even the most complex systems.

MultiWell is most suitable for time-dependent non-equilibrium systems. The real time needed for a calculation depends mostly upon the number of collisions during a simulated time period and on the number of stochastic trials needed to achieve the desired precision. For slow reaction rates and precise yields of minor reaction products, the code will require a long run time, but it will produce results. For long calculation runs, we often just let it run overnight.

MultiWell is a new code (1999) based on the Gillespie Exact Stochastic algorithm [1], as developed in our laboratory [2]. It will be described much more fully in a future publication.

For more information, see the MultiWell web site, or contact me.

-John R. Barker [jrbarker@umich.edu](mailto:jrbarker@umich.edu)

[1] (a) D. T. Gillespie, *J. Comput. Phys.*, 1976, 22, 403; (b) D. T. Gillespie, *J. Phys.*, 1977, 81, 2340; (c) D. T. Gillespie, *J. Comput. Phys.*, 1978, 28, 395.

[2] (a) J. R. Barker, *Chem. Phys.*, 77, 201 (1983). (b) J. Shi and J. R. Barker, *Int. J. Chem. Kinetics*, 22, 187 (1990). (c) J. R. Barker, *J. Phys. Chem.*, 96, 7361 (1992). (d) J. R. Barker and K. D. King, *J. Chem. Phys.*, 103, 4953 (1995).

### **Charge and Energy Transfer Dynamics in Molecular Systems**

We have the pleasure to announce the first edition of "Charge and Energy Transfer Dynamics in Molecular Systems" which will be published by Wiley-VCH in December 1999. This book emerged from lectures given to a Physics-Chemistry-Biology audience at different German universities during the last decade.

Writing the manuscript it has been our intention to provide a unified introduction into and a common interdisciplinary language for the theoretical treatment of various transfer phenomena in molecular systems.

The material spans the range from classical concepts to current areas of research in this field.

For further information please visit our homepage at

<http://userpage.chemie.fu-berlin.de/~manzwww/userpage/kuehn/book.html>

Volkhard May (Humboldt University Berlin), Oliver Kuehn (Free University Berlin)

**Theory and Application of Quantum Molecular Dynamics**

John Z.H. Zhang, 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/>