

# Molecular Dynamics News

number 93, February 1998

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 has been accepted - otherwise state *unpublished*).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@HERMES.CHM.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 94 to Prof. R. Anderson (You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#92). The closing date for issue number 94 is April 1, 1998.

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\*1998 Calendar-Year subscription for MDN, (six issues).

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

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

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# ANNOUNCING ELECTRONIC DELIVERY OF MDN

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

## 1. Electronic mail to subscribers

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

## 2. World Wide Web

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

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

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

### **The MDN e-mail list continues, as detailed below**

#### **MOLECULAR DYNAMICS NEWS EMAIL LIST**

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

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

join molecular-dynamics-news John F Kennedy

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

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

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

to the address mailbase@mailbase.ac.uk

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

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

join spectroscopy-group John Kennedy

## **a. Open Positions**

### **FACULTY**

#### **LECTURESHIP IN THEORETICAL AND COMPUTATIONAL CHEMISTRY, UNIVERSITY COLLEGE LONDON**

Applications are invited for the above position. The successful applicant will have a strong research interest and record of achievement in theoretical and computational chemistry. The salary will be on a point of the normal academic scale commensurate with age and experience, together with the London Allowance.

Applications (six copies, or one if from overseas) giving a full curriculum vitae, a detailed statement of an intended field of research, and the names and addresses of three referees, should be sent to: Professor R J H Clark FRS, Head of Department, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ.

The closing date for applications is 13 February 1998. Information on the department can be obtained from the web site <http://calcium.chem.ucl.ac.uk/webstuff/index.html>

Further details may be obtained from Professor David C. Clary FRS (same address as Prof. Clark, Tel 0171-391-1488; email: [d.c.clary@ucl.ac.uk](mailto:d.c.clary@ucl.ac.uk)).

### **POST DOCTORAL AND VISITING**

#### **POST-DOCTORAL RESEARCH ASSISTANTSHIP, PHYSICAL AND THEORETICAL CHEMISTRY LABORATORY, OXFORD UNIVERSITY**

Applications are invited for a research appointment, tenable for a period of 18 months, to work in collaboration with Professor J P Simons, Professor J M Brown and their research groups. The research project involves the use of laser induced fluorescence spectroscopy at rotational levels of resolution; one- and two-colour, mass-resolved resonantly enhanced ionisation spectroscopy; and the use of 'hole-burning' techniques, to probe the conformational landscapes of jet-cooled (bio)molecular systems. These include neuro-transmitters, amino-acids and simple peptides together with their hydrated clusters, and enzyme mimics. Applicants should be experienced in the use of pulsed and cw tunable dye laser systems and vacuum techniques and should be computer literate.

Starting salary, #16,927 p.a.; preferred starting date on or before February 1st 1998.

Applicants should submit a CV as soon as possible, identifying two referees, to Professor J P Simons FRS, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, England, FAX ++ 44 1865 275410, from whom further details may be obtained.

#### **POSTDOCTORAL, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD**

I wish to invite applications for postdoctoral research in my laboratory at NIST for quantitative and ultrasensitive laser-based gas analysis. The combination of NIST's unique mission to support industry, the depth of our personnel and our well-equipped facilities guarantees a rewarding postdoctoral research opportunity.

The appointments will be granted by the National Research Council for a period of two years. The starting salary is at least \$45,500/year, plus fringe benefits that include moving expenses, a professional travel allowance, and cost-shared health insurance. Awardees must be U.S. citizens and must have held a Ph.D. for less than 5 years.

As part of the application, the candidate must select a research project and submit a brief proposal.

Candidates are encouraged to contact me to discuss projects of mutual interest. I seek a candidate having a

strong desire to advance innovative research in a multi-disciplinary scientific program.

A list of possible project areas includes:

1. Cavity ring-down spectroscopy (CRDS) using cw diode lasers and pulsed systems
2. Tunable diode laser absorption spectroscopy (TDLAS)

The goals of this research are directed toward detection of stable species, radicals and ions for: semiconductor/plasma processing, environmental/emissions monitoring, humidity and atmospheric chemistry.

The applications must be postmarked by January 15, 1998. The final version of the proposal and letters of recommendation must be received at the NRC by February 15, 1998. Postdoctoral appointments will be announced in April 1998. Awardees may negotiate the starting date but must assume tenure by January 31, 1999. Application materials may be obtained directly from: Associateship Programs (TJ 2114), National Research Council, 2101 Constitution Avenue, N.W., Washington, D.C. 20418 (Tel. 202-334-2760, E-mail: rap@nas.edu).

Dr. Joseph T. Hodges, Process Measurements Division, Tel: 301-975-2605, Fax: 301-869-5924, E-mail: joseph.hodges@nist.gov, <http://fluid.nist.gov>

Note: for further information about applications including plasma and process diagnostics you may contact Dr. David S. Green old E-mail: dsgreen@enh.nist.gov, or new E-mail: david.green@nist.gov

### **EC IMAGINE Project - Postdoctoral Opportunities**

We are looking for 6 post-doctoral research associates with a variety of skills but in the overall field of chemical reaction dynamics with a particular emphasis on ion imaging and Rydberg atom tagging techniques.

The project, recently funded by the European Commission under the TMR programme, involves six laboratories: FOM (The Netherlands), Universitat Bielefeld (Germany), University of Bristol (UK), FORTH (Crete), University of Leeds (UK) and the University of Nijmegen (The Netherlands) with research groups headed by Win van der Zande (FOM), Peter Andresen (Beilefeld), Mike Ashfold (Bristol), Theo Kitsopoulos (FORTH), Ben Whitaker (Leeds) and Dave Parker (Nijmegen). The project also involves close collaboration with three industrial partners, El-Mul (Israel), LA Vision (Germany) and Photek (UK). Under the rules of the TMR programme you must be a European Community national or a national of one of the associated countries (Iceland, Israel, Leichtenstein or Norway) to be eligible for any one of these posts. Furthermore you may not be a national of the state of the laboratory to which you are applying. This is because the one of the aims of the TMR programme is to promote the exchange of young scientists between the states of the Community.

You may be expected to travel between the participating laboratories and our industrial partners but each PDRA will be primarily based in one site. Suitable candidates should apply to the following people for further details about the opportunities available in the various labs.

Wim van der Zande (zande@amolf.nl). The group at AMOLF are looking for someone to work primarily on photofragmentation studies of long lived metastable species and to develop novel high speed charge detectors and ion imaging experiments.

Peter Andressen (comet@physik.uni-bielefeld.de) wishes to develop high speed CCD camera technology for time slicing imaging experiments, and to continue their pioneering Rydberg tagging work, particularly in the context of bimolecular reaction dynamics.

Mike Ashfold (mike.ashfold@bristol.ac.uk) is interested in further extending the application of Rydberg atom tagging in studies of the primary photochemistry of hydride molecules, and of ion imaging methods for studying the photolysis of atmospherically relevant halogen containing species.

Theo Kitsopoulos (theo@luce.iesl.forth.gr). Crete plan ion-molecule reactive scattering experiments and also wish to develop high repetition rate molecular beam sources. The group also does ion imaging experiments with a particular emphasis on halogen containing species.

Dave Parker (parker@sci.kun.nl). The aim here is to develop imaging experiments for long lived metastable species and photoelectron and cation imaging coincidence experiments for photodissociation and reactions. Ben Whitaker (benw@chem.leeds.ac.uk) plans to use femtosecond laser systems to image dissociating systems in real time through Coulomb explosion experiments, and to develop existing ion imaging studies of photofragmentation.

The IMAGINE web page is at <http://www.chem.leeds.ac.uk/IMAGINE>. Links to the participating laboratories and the TMR programme pages can be found at this site.

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

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

The Femtosecond Science Program of the Steacie Institute for Molecular Sciences at the National Research Council of Canada (Ottawa) invites applications for post-doctoral research in the general area of:

Femtosecond Time-Resolved Photoelectron Spectroscopy.

NRC FEMTOSECOND SCIENCE PROGRAM, <http://gold.sao.nrc.ca/sims>, <http://www.femto.sims.nrc.ca>

Dr. P. B. Corkum, Group Leader, Adjunct Professor (McMaster); Dr. A. Stolow, Research Officer, Adjunct Professor (Queen's); Dr. D. M. Villeneuve, Research Officer, Adjunct Professor (INRS); Dr. M. Yu. Ivanov, Research Officer; Dr. D. M. Rayner, Research Officer, Adjunct Professor (Trent); A. G. Avery, Technical Officer; D. Joines, Technical Officer; J. Parsons, Technical Officer; D. Roth, Technical Officer.

We work in the general areas of:

Femtosecond Optics and Source Development:

- broadly tunable femtosecond infrared sources & applications
- high harmonic generation (femtosecond XUV & soft X-ray)
- attosecond (sub-femtosecond) pulse generation

Strong Field Physics:

- high power ultrashort pulses (10fs)
- strong field ionization of atoms & molecules
- time-resolved Coulomb explosion and applications

Coherent Control:

- strong field coherent control
- coherent optical phase control in isolated molecules and semiconductor devices

Time-resolved Molecular Dynamics:

- methods in femtosecond molecular dynamics

pump-probe photoelectron spectroscopy

pump-probe mass spectrometry

time-resolved product state distributions

- applications of wavepacket dynamics
- non-adiabatic (non-Born-Oppenheimer) wavepacket dynamics

We have modern state-of-the art laboratory facilities, excellent technical resources and combined experimental-theoretical research programs.

Interested persons (of any nationality) with a strong background in femtosecond optical sciences or molecular photoelectron spectroscopy should contact: [albert.stolow@nrc.ca](mailto:albert.stolow@nrc.ca)

Albert Stolow, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario CANADA K1A 0R6, TEL 613-993-7388, FAX 613-991-3437

### **POSTDOCTORAL POSITIONS, UNIVERSITY OF NOTRE DAME**

Three postdoctoral positions in Theoretical/Computational Chemistry are available immediately in the Hammes-Schiffer research group in the following areas:

1. Investigation of proton and hydride transfer reactions in enzymes using mixed quantum/classical molecular dynamics methods
2. Investigation of (a) photochemical reactions in solution or (b) solvation dynamics of fundamental organic reactions
3. Investigation of proton-coupled electron transfer reactions in solution using mixed quantum/classical molecular dynamics methods

These projects involve a combination of method development and applications. Computer programming experience and a strong background in physical chemistry and/or chemical physics are required. The positions are available immediately, but the exact starting date is flexible. The expectation is that the position will be for two years, subject to renewal upon mutual agreement after the first year.

See my web site <http://www.nd.edu/shammes> for more information.

Please send CV and at least 2 letters of recommendation to:

Professor Sharon Hammes-Schiffer, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, USA, Telephone: (219) 631-7434, e-mail: [hammes-schiffer.1@nd.edu](mailto:hammes-schiffer.1@nd.edu)

#### **POSTDOCTORAL POSITIONS IN CHEMICAL DYNAMICS, ACADEMIA SINICA, TAIWAN**

Two postdoctoral positions are to be filled in the chemical reaction dynamics laboratory in Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica, Taiwan, ROC. Successful candidates will be working in photodissociation and crossed molecular beam reaction experiments using VUV lasers and/or VUV synchrotron radiations as the probing techniques. The VUV laser beams will be generated using difference frequency mixing in Kr gas. VUV synchrotron radiation will be provided by a 3rd generation synchrotron radiation facility in Hsingchu, Taiwan.

Qualified candidates with experience with pulsed lasers and molecular beams are encouraged to apply. The starting salary of the positions will be about US\$2000 per month, plus a one way ticket to Taiwan. Interested candidates should send C.V. to Dr. Xueming Yang, P. O. Box 23-166, Institute of Atomic and Molecular Sciences, Academia Sinica, E-mail: [xmyang@po.iams.sinica.edu.tw](mailto:xmyang@po.iams.sinica.edu.tw), Fax: 886-2-3691638

#### **POSTDOCTORAL POSITION, INSTITUTE FOR MOLECULAR SCIENCE, OKAZAKI, JAPAN**

Two postdoctoral positions are available immediately in the group of Professor Toshinori Suzuki at the Institute for Molecular Science in Okazaki, Japan. Research projects involve, (i) femtosecond pump-probe experiments on molecular photodissociation, (ii) dynamical stereochemistry in molecular photodissociation, and (iii) crossed beams study on fundamental atmospheric reactions.

A solid-state high power femtosecond laser, high vacuum molecular beam machines, and a crossed beams apparatus equipped with 2D imaging device are in operation in these projects. Housing at our guest house is offered, and various assistance is given by a secretary for foreign researchers at IMS. The appointment is for at least one year and is renewable. More information about IMS can be found at <http://www.ims.ac.jp>.

Recent publications from the group can be found in, for example, JPC A, 101, 7754 (1997), JPC A, 101, 6697(1997), JCP, 106, 5292(1997), and PRL, 77, 830 (1996).

Successful candidates with good knowledge of reaction dynamics and some experience with molecular beams and/or laser spectroscopy are encouraged to apply. Candidates should arrange two letters of recommendation, a CV, and a list of publications sent to: Professor Toshinori Suzuki, Institute for Molecular Science, Okazaki National Research Institutes, Myodaiji, Okazaki, 444 Japan, E-mail: [suzuki@ims.ac.jp](mailto:suzuki@ims.ac.jp), FAX 81-564-54-2254

#### **POSTDOCTORAL POSITION, SUNY COLLEGE OF ENVIRONMENTAL SCIENCE AND FORESTRY**

There is an opening in my laboratory for a postdoctoral research associate to lead a project: "Spectroscopy and Unimolecular Reactions of Alkoxy Radicals." The position would start around May of 1998. Alkoxy radicals (RO) are important intermediates in the degradation of volatile organic compounds in the lower

atmosphere. The electronic spectroscopy of alkoxy radicals will be studied by LIF, and their rates of unimolecular reaction determined.

The successful candidate should have a Ph.D. by the starting date and significant experience with pulsed lasers and electronic spectroscopy. Experience in kinetics and atmospheric chemistry is not required. This project represents an excellent opportunity to learn about atmospheric chemistry and about important problems in that field that can be addressed by basic research.

The Chemistry Department at SUNY-ESF offers a Ph.D. program in chemistry and is in the process of moving into a brand new Chemistry Building. We have access to all the facilities of Syracuse University, located just across the street, including their fine library system.

Preliminary inquiries can be sent to me at [tsdibble@mailbox.syr.edu](mailto:tsdibble@mailbox.syr.edu). Some general information on my research plans, the department, the College, and the area can be obtained through my web page at [www-chem.esf.edu/info/faculty/dibble/dibble.htm](http://www-chem.esf.edu/info/faculty/dibble/dibble.htm) and the College web page [www.esf.edu](http://www.esf.edu). Applicants should send a CV and arrange for three letters of recommendation to be sent to me.

Theodore S. Dibble, Department of Chemistry, SUNY College of Environmental Science and Forestry, One Forestry Drive, Syracuse NY 13210, Telephone: (315) 470-6596, FAX: (315) 470-6856, E-mail: [tsdibble@mailbox.syr.edu](mailto:tsdibble@mailbox.syr.edu)

### **POSTDOCTORAL RESEARCH, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD**

The postdoctoral research in cavity ring-down spectroscopy, will concentrate on applications to Chemical Reactions on Thin Films, to Gas-liquid Interactions, to Heterogeneous Chemistry at Interfaces, to Solution-phase Photochemistry, to Gas-Phase Radical-radical Reaction Systems, and on Fundamental Aspects of CRDS Applications within the Experimental Chemical Kinetics and Thermodynamics Group at the National Institute of Standards and Technology (Gaithersburg, MD). An informative web-page on the recent developments that have made our unique opportunities possible is found at:

[http://www.nist.gov/cstl/div838/crds\\_web/](http://www.nist.gov/cstl/div838/crds_web/)

The Postdoctoral research will be conducted under the auspices of the National Research Council (NRC). These positions are competitively awarded on the bases of a research proposal, transcripts, and letters of recommendation. More program details are available through our websites.

THE SALIENT FEATURES OF THE NIST-NRC PROGRAM ARE:

ELIGIBILITY: US citizens holding a Doctorate for less than five years. APPLICATION DEADLINE:

January 15, 1998 BEGIN TENURE: Negotiable, ordinarily after Oct 1, 1998 and by Feb 1, 1999. LENGTH OF TENURE: Two years. ANNUAL SALARY: \$47,000. BENEFITS: Moving expenses, health plan, professional travel allowance.

Additional information about our research and about NIST is available through the webpages at

[http://www.nist.gov/cstl/div838/group\\_04/experkin\\_838\\_04.html](http://www.nist.gov/cstl/div838/group_04/experkin_838_04.html)

Contact:

Jeffrey W. Hudgens, [Hudgens@nist.gov](mailto:Hudgens@nist.gov), Tel. 301-975-2512

[http://www.nist.gov/cstl/div838/group\\_04/staff/hudgens/welcome\\_jwh.html](http://www.nist.gov/cstl/div838/group_04/staff/hudgens/welcome_jwh.html)

Robert E. Huie, [Huie@nist.gov](mailto:Huie@nist.gov), Tel. 301-975-2559

[http://www.nist.gov/cstl/div838/group\\_04/staff/huie/huie\\_homepage.html](http://www.nist.gov/cstl/div838/group_04/staff/huie/huie_homepage.html)

### **POSTDOCTORAL RESEARCH IN LASER APPLICATIONS, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD**

We would like to call your attention to postdoctoral research opportunities with the Laser Applications Group at the National Institute of Standards and Technology, located just outside Washington, D.C. The group emphasizes interdisciplinary research in selected areas of photophysics, photochemistry, and optics. We are looking for postdocs to work on projects in several areas, including ultrafast laser studies of

dynamical processes in gases, liquids, solids, and at interfaces; linear and nonlinear light-scattering interactions as probes of surface and interfacial structure; and measurements of the near-field optical properties of nanometer-scale structures.

Positions will be filled on a competitive basis through the NIST-National Research Council Postdoctoral program, with starting salaries of \$47,000. Prospective postdocs must be U.S. citizens, available to start during the period July 1998 through January 1999, and must submit a research proposal. More information on the NIST-NRC program, application forms, and a booklet which describes all postdoctoral research opportunities at NIST, are available on request from the NRC, telephone number (202) 334-2760, and also at <http://rap.nas.edu/lab/NIST>. The deadline for completed application materials is January 15, 1998.

Additional information about the group and about NIST is available on our web pages at <http://physics.nist.gov/lag>. Prospective postdocs are encouraged to contact us immediately.

M. P. Casassa, [mcasassa@nist.gov](mailto:mcasassa@nist.gov), (301)975-2371

T. A. Germer, [tgermer@nist.gov](mailto:tgermer@nist.gov), (301)975-2876

L. S. Goldner, [lgoldner@nist.gov](mailto:lgoldner@nist.gov), (301)975-3792

E. J. Heilweil, [eheilweil@nist.gov](mailto:eheilweil@nist.gov), (301)975-2370

J. C. Stephenson, [jstephenson@nist.gov](mailto:jstephenson@nist.gov), (301)975-2372

### **POSTDOCTORAL POSITION, UNIVERSITY OF BASEL**

A Postdoctoral position is available with John P.Maier's group at the Institute of Physical Chemistry, University of Basel, Switzerland to participate in the project to characterize carbon chains and clusters by their electronic spectra in neon matrices. The approach which has been developed is based on codeposition of mass-selected ion beams with neon to form a matrix at 5 K, and has been used successfully in the recent years to study species with up to twenty carbon atoms. The Postdoc appointed is expected to extend and apply this approach for the larger carbon species. Experience in experimental chemical physics is required. The starting date is negotiable (after 1.January 1998) and the salary in the first year is around SFr. 50000, depending on qualifications and previous experience.

Interested applicants should contact: Professor J.P.Maier, Institute of Physical Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland. Tel. +41 61 267 38 26, Fax. +41 61 267 38 55, Email: [MAIER@UBACLU.UNIBAS.CH](mailto:MAIER@UBACLU.UNIBAS.CH)

### **POSTDOCTORAL POSITION AT THE UNIVERSITY OF FLORIDA ON QUANTUM MOLECULAR DYNAMICS**

A postdoctoral associate position will be available in the research group of David Micha starting in January, 1998, or later. It involves work on first principles quantum molecular dynamics, and its applications to interactions in the gas phase, in clusters, and at solid surfaces. The applicant should have experience on molecular dynamics and the use of electronic structure computational software. Familiarity with Fortran, Unix OSs and good communication skills are desirable. The position is for a year, extended to two years by mutual agreement. The applicant should submit to the address below a CV listing experience, publications and presentations. Please send the names, phone and FAX numbers, and e-mail of two references.

The work will be done at the Quantum Theory Project, an institute for theory and computation in molecular and materials sciences with 11 Faculty members in Chemistry and Physics, over 60 people involved in scientific research, and excellent computing facilities.

Some related recent work may be found in Chem. Phys. Lett. 256, 321 (1996), Phys. Rev. A53, 1388 (1996), J. Chem. Phys. 103, 3795 (1995), and J. Chem. Soc. Faraday Trans. 93, 969 (1997). More details on research areas are given in the home page

<http://www.qtp.ufl.edu/micha> .

Please contact: Prof. David A. Micha, P.O. Box 118435, 366 Williamson Hall, University of Florida, Gainesville FL 32611-8435, tel. 352-392-6977, e-mail: [micha@qtp.ufl.edu](mailto:micha@qtp.ufl.edu)

### **POSTDOCTORAL POSITION AT FOM IN AMSTERDAM**

Qualified candidates are encouraged to apply for a postdoctoral position which is available in the XUV physics group of the FOM Institute for Atomic and Molecular Physics in Amsterdam (The Netherlands). The successful candidate will participate in experiments where femtosecond extreme ultra-violet (XUV) laser pulses which are produced via High Harmonic Generation are used in time-resolved (pump&probe) experiments.

In one experiment, the photodissociation dynamics of polyatomic molecules is studied in both the time- and the frequency-domain by carrying out a femtosecond pump-probe experiment in combination with 2-dimensional ion imaging detection. In another experiment, photoionization processes are studied with (sub)-picosecond time-resolution, using an ultrafast streak camera developed at the institute.

We strongly encourage candidates with a background in molecular reaction dynamics and/or ultrafast laser techniques to apply. The initial appointment will be for a period of one year.

For further information please contact:

Dr. Marc Vrakking, Projectleader XUV physics, Tel: (020)-6081349, FAX: (020)-6684106, E-mail: vrakking@amolf.nl

Or send your application including curriculum vitae & list of publications to:

Prof.dr. J.T.M. Walraven, Director FOM Institute AMOLF, Kruislaan 407, 1098 SJ Amsterdam

### **RESEARCH ASSOCIATE, CORNELL UNIVERSITY DEPARTMENT OF CHEMISTRY**

A Research Associate position in physical chemistry with specific expertise in molecular reaction dynamics is available with Paul Houston in the Department of Chemistry at Cornell University commencing during the first three months of 1998. Duties are conducting experiments on the laser photodissociation of radicals and state-selected molecules, conducting experiments on reactions in crossed molecular beams probed by laser and imaging techniques, and assisting in the administration of a research group of 10 graduate students and postdoctoral associates. A Ph.D. in physical chemistry or chemical physics is required and at least two years of research experience past the Ph.D. is expected. Experience with nanosecond pulsed excimer- and YAG-pumped dye lasers, pulsed molecular beams, high vacuum equipment, and timing and data acquisition electronics is essential. Interested candidates should send a curriculum vitae and arrange for three letters of recommendation to be sent to Paul L. Houston, Baker Laboratory of Chemistry, Cornell University, Ithaca, NY 14853-1301 U. S. A. The annual salary is \$33,000. The deadline for applications is October 15, 1997. Cornell University is an Affirmative Action/Equal Opportunity Employer and Educator.

See: <http://www.msc.cornell.edu/plh2/group/plhhome.html>

### **POSTDOCTORAL POSITION, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, TAIWAN**

A post doctoral position is available in the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, ROC. The primary mission of the successful candidate is to investigate the chemical dynamics and reaction products of neutral-neutral reactions relevant to the chemistry in the atmosphere of Saturn's moon Titan employing crossed molecular beams experiments. The results of these investigations are expected to play a significant role to understand data of the Cassini probe - a Saturn bound spacecraft analyzing Titan's atmosphere. Interested candidates should send CV and two reference letters to:

Dr. Ralf I. Kaiser, Institute of Atomic and Molecular Sciences, Academia Sinica, 1 Section 4, Roosevelt Rd., Taipei, 106, Taiwan, ROC. Tel: 886-2-3645370; Fax:886-2-3620200; email: kaiser@po.iam.sinica.edu.tw.

### **POSTDOCTORAL POSITION IN PHYSICAL CHEMISTRY AT THE UNIVERSITY OF UTAH**

A new post-doctoral position will be available in the laboratories of W. H. Breckenridge, Department of Chemistry, University of Utah beginning July 1, 1998. The position, funded by the Petroleum Research Foundation, will involve innovative studies of C-H and C-F bond activation in the gas phase, by laser excitation of excited states of metal atoms or of metal-oxide molecules within van der Waals complexes

("full-collision" studies are also planned). The experiments will be performed in a sophisticated supersonic-jet/molecular-beam apparatus in which various preparative sources can be utilized, and both LIF and R2PI characterization of the complexes or photo-products will be possible. Candidates with outstanding experimental expertise in gas-phase spectroscopy, LIF, R2PI, and/or molecular beam techniques will be given preference. Salary will be \$26,000 per year, and full medical and dental insurance coverage will be provided for the Fellow and any immediate family members. The position will be for one year initially, with an extension to two years possible by mutual consent. Applicants should send (by March 1st) their curriculum vitae and have three letters of reference sent directly from the referees to: Prof. W. H. Breckenridge Dept. of Chemistry, University of Utah, Salt Lake City, Utah 84112, USA e-mail: breckenridge@chemistry.utah.edu Fax: 801-581-8433

#### **POSTDOCTORAL RESEARCH ASSOCIATE POSITION, THE UNIVERSITY OF CHICAGO**

Postdoctoral Research Associate position available for conducting experimental studies of the structures of the various interfaces between a liquid metal (or alloy) and another medium (vapor, wall, solution) using a variety of x-ray based methods, e.g., grazing incidence x-ray diffraction, x-ray reflectivity, anomalous diffraction and reflectivity, etc. This position is available for immediate appointment. Interested individuals should contact: Prof. Stuart A. Rice, James Franck Institute The University of Chicago 5640 S. Ellis Avenue Chicago, IL 60637

TEL: 773 702 7199, FAX: 773 702 5863 e-MAIL: sarice@rainbow.uchicago.edu

Please include a cv and name two references who know your work and are willing to write a letter of recommendation.

#### **POSTDOCTORAL RESEARCH ASSOCIATES IN INTERFACIAL SCIENCE**

Applications are invited for three research associateships on EPSRC funded research projects in: (i) Condensed phase laser cooling

(ii) Scanning probe microscopy of nanoparticles

(iii) New electrocatalysts for oxygen reduction.

Candidates must have a PhD in Physical Chemistry, Chemical Physics or Physics. Appointments are for one year initially, with the possibility of extending to three years. Salary will be on the RA1A scale + London allowance. Applicants should send a CV with the names of two referees by 28th February 1998 to: Mrs.L.Ainsworth, Interfacial Science Group, Department of Chemistry, Imperial College, London, SW7 2AY, UK.

Further information can be found at <http://www.ch.ic.ac.uk/jobs/>

#### **POSTDOCTORAL RESEARCH ASSISTANTSHIP, UNIVERSITY OF SUSSEX**

A Postdoctoral Research Assistantship is available at Sussex University for work in collaboration with Prof. A.J. Stace on gas phase studies of the magnetic and electronic properties of small metallic clusters. This position is available immediately and is funded for two years through the Advanced Magnetics Initiative of EPSRC. Applicants should have a background in either Chemical Physics or Physics and have some experience of vacuum techniques, molecular beam methods, or low temperature techniques. Applicants should send a CV and the names of two referees to Prof. A.J. Stace, School of Chemistry, Physics and Environmental Sciences, University of Sussex, Falmer, Brighton BN1 9QJ, U.K.

Further details can be obtained by contacting: a.j.stace@sussex.ac.uk.

#### **POSTDOCTORAL POSITION IN LASER SPECTROSCOPY OF ORGANIC MOLECULES**

I am looking for a post-doc interested in doing one- and two-color REMPI, as well as some vuv PFI/ZEKE, studies on organic molecules such as cyclic ketones, ethers, etc. as well as straight chain saturated molecules. The object is to determine conformations of floppy molecules cooled to a few degrees Kelvin. One of the unique features of our experiment is a variable temperature pulsed valve which permits us to vary

the equilibrium concentrations of the various conformations (axial-equatorial or ethyl rotor orientations) prior to valve expansion. A recent feature article in the J. Phys. Chem. [101: 8970-8 (1997)] gives some background information about this project. The successful candidate should have experience with pulsed lasers, 2-color experiments, and/or vuv laser generation. Two letters of recommendation and a resume should be sent to Prof. Tomas Baer. Starting time is anytime after April 1, 1998. Tomas Baer Kenan Professor of Chemistry Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290. Phone: 919 962 1580, Fax: 919 962 2388, Baer@unc.edu <http://net.chem.unc.edu/faculty/tb/cftb01.html>

### **POSTDOCTORAL POSITIONS AT AFRL HANSCOM AFB, MA**

Postdoctoral research positions are available at the Air Force Research Laboratory at Hanscom Air Force Base, near Boston, Massachusetts. The research is conducted in an academic style and results are published in the open literature.

There are postdoctoral positions available in the COCHISE (COld CHEMical Simulation Experiment) facility of the Air Force Research Laboratory at Hanscom AFB, Massachusetts. Experimental research in chemical physics is performed in order to more fully understand the chemistry and physics of the atmosphere, especially in relationship to the production of infrared radiation in the thermosphere. Examples of research include the spectroscopy and kinetics of fast nitrogen atom collisions with oxygen molecules [fast  $N + O_2 \rightarrow NO(v, highJ) + O$ ] where both the precursors and the details of the very highly rotationally excited states of NO will be investigated. In addition, the quenching of NO and OH vibrational and rotational energy by a variety of atmospheric species both at room temperature and at thermospheric temperatures (700 - 1500 K) is an active area of study. Please contact Steven Miller, phone (781)377-2807 or email [miller@plh.af.mil](mailto:miller@plh.af.mil) for further information.

Postdoctoral research positions are available at the Air Force Research Lab's LABCEDE (Laboratory Cryogenic Energy Deposition Experiments) facility at Hanscom Air Force Base, outside Boston, Mass. Several research areas in chemical physics are currently being pursued, including laboratory experiments that simulate uv and electron irradiation processes in the upper atmosphere, and analysis of infrared atmospheric spectra from space-based experiments. Specific topics include the measurement of collisional deactivation rates of highly rotationally excited diatomic molecules, and the analysis of rotational and vibrational excitation in OH formed by the  $H + O_3 \rightarrow OH + O_2$  reaction. Equipment on hand includes a cryogenic-temperature atmospheric simulation chamber, high resolution Michelson interferometers, and a number of pulsed and cw lasers. Data acquisition is based on TRFTS (time-resolved Fourier transform spectroscopy), and extensive computer facilities are available for data analysis and numerical modeling. For information, contact Dr. Steven Lipson at [lipson@plh.af.mil](mailto:lipson@plh.af.mil) or at (781) 377-3626.

For the above positions is required U.S. citizenship or permanent resident status.

### **POSTDOCTORAL POSITION, UNIVERSITY OF ILLINOIS**

There is a postdoctoral associate position available immediately in the research group of Prof. Jim Lisy at the University of Illinois. Individuals with interests (or experience) in mass spectrometry and/or infrared spectroscopy, would be able to make an immediate impact. Our research group has been at the forefront of research on ionic clusters, using mass-selective infrared spectroscopy and Molecular Dynamics/Monte Carlo simulation methods. Our laboratory is well-equipped with multiple ion cluster machines and tunable infrared laser sources. In addition, we have two SGI workstations: an Indigo 2, and a dual processor Octane, for the simulation studies. We are presently expanding our capabilities to study larger clusters, as well as multiply-charged ions. Of particular interest are systems which exhibit size-selective binding or conformations. The initial appointment is for one year, but funds are available for extension based upon mutual agreement.

Applicants should arrange to send their C.V.'s to the address below using conventional or electronic mail. Names and addresses of two to three references should also be provided at this time. Professor James M.

Lisy, Department of Chemistry Box 7-6, University of Illinois at Urbana-Champaign, 600 South Mathews Ave. Urbana, IL 61801 USA email: j-lisy@uiuc.edu phone: (217)333-2898 FAX: (217)244-3186

### **POSTDOCTORAL POSITION AT THE TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY**

A postdoctoral position is available immediately in the research groups of Izhack Oref and Israel Schechter, at the department of chemistry. The research is focused on experimental physical and analytical aspects of sonochemistry. Information on the Department can be found at

<http://www.technion.ac.il/technion/chemistry/>. Applicants with strong background in modern spectroscopy, including operation of ICCD detectors, will be given preference. Please send CV listing experience and publications as well as the names, telephone and fax numbers and e-mail addresses of two references to the addresses below. In addition, please request references to forward letters to the following addresses.

Professor Izhack Oref, Department of Chemistry, Technion - IIT Haifa 32000, ISRAEL, Fax: (972) 4

8293643; Dr. Israel Schechter, Department of Chemistry, Technion - IIT Haifa 32000, ISRAEL Fax: (972) 4 8293643

### **POST-DOCTORAL POSITIONS IN BERKELEY**

Opportunities are available on the new Chemical Dynamics Beamline at the Advanced Light Source to study reaction dynamics and photochemistry of radicals. This unique User Facility

(<http://www.lbl.gov/chemicaldynamics>) features a 10cm undulator providing  $1e16$  VUV photons/second continuously tunable from 5 to 30 eV, along with dedicated molecular beam endstations using both neutral time-of-flight as well as ion imaging detection methods.

Successful candidates will be expected to develop new radical molecular beam sources; perform studies of radical photochemistry and crossed-beam reaction dynamics; develop innovative applications of synchrotron radiation to chemical dynamics studies such as coincidence imaging studies of neutral photochemistry; perform collaborative studies with outside users; publish results in recognized journals. These positions require a PhD in Chemical Physics or a related discipline, experience in molecular beam photochemistry or reaction dynamics studies and a record of publication in chemical dynamics or a closely related field.

Experience with synchrotron radiation is useful but not necessary. Interested applicants should send a CV and arrange for two letters of recommendation (email preferred) to:

Dr. Arthur G. Suits, Chemical Dynamics Group, MS 10-118 E. O. Lawrence Berkeley National Laboratory Berkeley CA 94720 USA

Tel +1 510-486-4754 Fax +1 510-486-5664 Internet [agsuits@lbl.gov](mailto:agsuits@lbl.gov) <http://www.lbl.gov/agsuits>

## **b. Preprints**

### **A combined crossed molecular beams and ab initio investigation on the formation of carbon-bearing molecules in the ISM via neutral-neutral reactions**

J. Chem. Soc. Faraday Disc.(submitted)

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

Academia Sinica, Institute of Atomic and Molecular Sciences, 1, Section 4, Roosevelt Rd., Taipei, 116, Taiwan, ROC; Departments of Chemistry, University of California, Berkeley, California, 94720, USA

Results of the crossed molecular beams reactions  $C(^3P_j) + H_2S$ ,  $C(^3P_j) + H_2CCCH_2$ ,  $C(^3P_j) + C_2HD$ , and  $C(^3P_j) + C_2H_3$  combined with electronic structure calculations are presented. The relevance of each reaction with respect to interstellar chemistry is discussed.

### **Fourier transform millimeter-wave spectroscopy of the HCS radical in the $^2A'$ ground electronic state**

Journal of Chemical Physics (submitted)

H.Habeta, S. Yamamoto, C. Ochsenfeld, M. Head-Gordon, R.I. Kaiser, Y.T. Lee

Department of Physics, The University of Tokyo, Bunkyo-ku, Tokyo 119, Japan; Department of Chemistry,

University of California, Berkeley, California, 94720, USA; Academia Sinica, Institute of Atomic and Molecular Sciences, 1, Section 4, Roosevelt Rd., Taipei, 116, Taiwan, ROC.

The 1(01)-0(00) rotational transitions of the HCS radical in the  $X^2A'$  ground electronic state has been observed with a Fourier transform millimeter wave spectrometer with a pulsed discharge nozzle. Six fine and hyperfine components are detected, and the effective rotational constant, spin-rotation interaction constant, hyperfine interaction constants are determined accurately.

### **Phase Conjugation Through Four-Wave Mixing**

Computational Studies of New Materials Edited by D. A. Jelski and T. F. George (World Scientific, Singapore, 1998)

Henk F. Arnoldus and Thomas F. George\*

Office of the Chancellor Departments of Chemistry and Physics & Astronomy, University of Wisconsin-Stevens Point Stevens Point, WI 54481-3897 tgeorge@uwsp.edu

A numerical study is reported for the situation where a nonlinear crystal is illuminated by two strong counterpropagating laser beams, such that the medium acquires the potential for generating a phase-conjugated replica of a weak incident field through the mechanism of four-wave mixing.

### **Viscosity and Ultrasonic Attenuation in $^4\text{He}$ below 0.6 K**

Low Temperature Physics

Chung-In Um, Soo-Young Lee, Sahng-Kyoon Yoo, Thomas F. George,\* Lakshmi N. Pandey and Igor N. Adamenko

Office of the Chancellor Departments of Chemistry and Physics & Astronomy, University of Wisconsin-Stevens Point, Stevens Point, Wisconsin 54481-3897, tgeorge@uwsp.edu

Through a treatment of three-phonon processes, wide-angle scattering rates and absorption rates of phonons, which characterize viscosity and ultrasonic attenuation, respectively, are calculated.

### **The formation of HCS and HCSH molecules and their role in the collision of comet Shoemaker-Ley 9 with Jupiter**

Science

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

Department of Chemistry, University of California, Berkeley, CA 94720, USA.

The reaction of hydrogen sulfide with ground state atomic carbon was examined in crossed molecular beams experiments and ab initio calculations. The thiohydroxycarbene molecule, HCSH, was the reactive intermediate which fragmented into atomic hydrogen and the thioformyl radical, HCS. This finding may account for the unassigned HCS source and an unidentified HCSH radical needed to match observed CS abundances from the collision of comet Shoemaker-Levy 9 into Jupiter. In the shocked jovian atmosphere, HCS can further decompose to H and CS, and CS can react with SH and OH to yield observed  $\text{CS}_2$  and COS.

### **Rotational quenching of dipole-dipole interaction**

Europhysics Letters 38 (1997) 503

E.J. van Duijn, G. Nienhuis and L.J.F. Hermans

Huygens Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

Rotational-state-dependent cross sections for HF with Ar,  $\text{H}_2$ , HCl,  $\text{CH}_4$  and  $\text{CH}_3\text{F}$  were measured and the strong J-dependence for dipolar systems compared with a Born approximation treatment.

### **Rotational- and vibrational-state resolved HF-surface interactions investigated by surface light-induced drift**

J. Chem. Phys. 107 (1997) 3999

E.J. van Duijn, R. Nokhai, L.J.F. Hermans, A.Yu. Pankov and S.Yu. Krylov

Huygens Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

Experiments based on tangential momentum accommodation measurements yield information on the rotational- and vibrational-state-dependent molecule-surface interaction.

### **Quantum Zeno Effect Induced by Collisions**

Phys. Rev. Letters 79 (1997) 3097

B. Nagels, L.J.F. Hermans and P.L. Chapovsky

Huygens Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

Under appropriate conditions the ortho-para conversion rate of gaseous CH<sub>3</sub>F is measured to decrease with increasing pressure. This 1/p behavior is interpreted as a manifestation of the Quantum Zeno Effect where the perturbation caused by collisions may be regarded as a measurement.

### **Nuclear spin conversion in CH<sub>3</sub>F at elevated temperatures**

Phys. Rev. A (1998)

B. Nagels, P. Bakker, L.J.F. Hermans and P.L. Chapovsky

Huygens Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

The ortho-para conversion rate of <sup>12</sup>CH<sub>3</sub>F is found to increase as a function of temperature, while that for <sup>13</sup>CH<sub>3</sub>F decreases sharply. This is in qualitative agreement with a conversion mechanism based on mixing of states.

### **Reactive scattering of ground-state and electronically excited oxygen atoms on a liquid hydrocarbon surface**

Faraday Discussion 108, 000 (1997)

Donna J. Garton, Timothy K. Minton\*

Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT 59717, USA

Michele Alagia, Nadia Balucani, Piergiorgio Casavecchia and Gian Gualberto Volpi

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

The dynamics of initial oxygen-atom reactions at a saturated hydrocarbon surface were studied by directing an O-atom beam at a continuously refreshed liquid squalane surface and monitoring energy and angular distributions of the volatile reaction products.

### **Crossed molecular beams and quasiclassical trajectory studies of the reaction O(<sup>1</sup>D)+H<sub>2</sub>(D<sub>2</sub>)**

J. Chem. Phys. (1998)

M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia\*, E.H. van Kleef, G.G. Volpi

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

P.J. Kuntz

Hahn-Meitner-Institute für Kernforschung Berlin, D 1000 Berlin, Germany

J.J. Sloan

Department of Chemistry, University of Waterloo, Waterloo, Canada N2L 3G1

The dynamics of the reactions O(<sup>1</sup>D)+H<sub>2</sub> → OH+H and O(<sup>1</sup>D)+D<sub>2</sub> → OD+D have been investigated in crossed molecular beam experiments with mass spectrometric detection at the collision energies of 1.9 and 3.0 kcal/mol, and 5.3 kcal/mol, respectively. The results are compared with quasi-classical trajectory calculations on a DIM potential energy surface.

### **Magnetic analysis of supersonic beams of atomic oxygen, nitrogen, and chlorine generated from a radio-frequency discharge**

Israel J. Chem. (special issue on Molecular Beams)

M. Alagia, V. Aquilanti, D. Ascenzi, N. Balucani, D. Cappelletti<sup>a</sup>, L. Cartechini, P. Casavecchia, F. Pirani, G. Sanchini and G.G. Volpi

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

<sup>a</sup> Istituto per le Tecnologie Chimiche, Università di Perugia, 06125 Perugia, Italy

Supersonic beams of oxygen, nitrogen, and chlorine atoms and of metastable oxygen and nitrogen molecules produced

from a high-pressure radio-frequency discharge beam source have been characterized by coupling velocity selection with Stern-Gerlach magnetic analysis.

### **Evidence For Hybrid Classical-Quantal Behaviour in State and Angle Resolved Atom-Diatom Scattering**

J. Phys. B At. Mol. Opt. Phys. 30, 5773 (1997)

Anthony J. McCaffery and Ruth J. Wilson

School of Molecular sciences, University of Sussex, Brighton BN19QJ, Sussex, U.K.

A new spectroscopic technique for obtaining state to state angular distributions of molecules in ground states allows comparison of results with molecular beam methods. A good correlation is found. These and previously published scattering angles on a wide range of collision systems all obey a modified Newtonian vector relationship in which the perpendicular component of velocity just opens the channel and the parallel component is scattered. This is termed quantum constrained kinematics since the Newtonian mechanics is constrained by the internal quantum structure of the molecule.

### **Atom-Diatom Collisions in the Momentum Space Representation; a Connection Between Quantum and Classical Expressions.**

J. Phys. B At. Mol. Opt. Phys.

Thomas W.J. Whiteley, Anthony J. McCaffery and K. Truhins

School of Molecular Sciences, University of Sussex, Brighton BN19QJ, Sussex, U.K.

The impulsive collinear collision of an atom and diatom is expressed in the momentum space representation. We find an interesting connection between classical and quantal picture (assuming the diatomic oscillator to be quantised) and a faster convergence in the quantum numerical solution. The representation also provides an analytical approximation for systems initially in their ground states that is analogous to the Franck-Condon overlap integral of spectroscopy .

### **On the exact analytical formulation of atomic scattering from a hard hemisphere on a flat and rigid surface.**

J. Chem. Phys. (submitted)

Didier Lemoine

LDMP, URA 779, Universite de Lille 1, Batiment P5, 59655 Villeneuve d'Ascq, France

### **Atomic scattering from single adsorbates: what can we learn from gas phase ?**

Phys. Rev. Lett. (submitted)

Didier Lemoine

LDMP, URA 779, Universite de Lille 1, Batiment P5, 59655 Villeneuve d'Ascq, France

Within an adsorbed hemisphere model one can unambiguously assign the first interference peaks of the exact angular distribution of He scattering from CO on a metal surface, to be gas phase-like features such as rainbow and Fraunhofer diffraction effects.

## **c. Conferences**

### **1. CCP6 WORKSHOP ON FASHIONING A MODEL: OPTIMIZATION METHODS IN CHEMICAL PHYSICS**

Collingwood College, Durham (England): 24 - 27 March 1998

Physical models often contain adjustable parameters, which must be determined from experimental and/or theoretical considerations. Examples in chemical physics include the determination of potential energy surfaces from either experimental data or ab initio points, the analysis of spectra, and the determination of structural parameters. However, the optimization process is fraught with difficulties, and there is often no formally unique solution: instead, the scientist applies physical insight to discriminate between different possible models, to choose the degree of flexibility to include, and to keep the parameter values within

physically sensible limits. Scientists in different fields have evolved their own ways of choosing models and guiding the progress of the optimisation. The purpose of the workshop will be to bring people working on "difficult" optimisation problems in different fields together so that they can pool their expertise and learn from one another's experience. The workshop will run for two and a half days, convening on the evening of Tuesday 24 March and ending at lunchtime on Friday 27 March. There will be about 10 invited speakers. Afternoons will be kept free as far as possible for individual discussions. An online registration form is available at <http://www.dur.ac.uk/dch3njw/form.html>

The workshop is sponsored by CCP6, the EPSRC Collaborative Computational Project on Heavy Particle Dynamics. It will be a small meeting, with about 12 invited talks and a poster session. We intend to limit the size to about 30-40 keenly interested participants. The format will be "Gordon Conference style", with sessions in the morning and evening but afternoons free. Invited speakers at the workshop are expected to include:

Robert J. Le Roy (Waterloo), Herschel Rabitz (Princeton), Mark M. Law (Aberdeen), Ian M. Mills (Reading), Anthony J. Stone (Cambridge), Julius Jellinek (Argonne), Joel M. Bowman (Emory), Peter Willett (Sheffield).

CCP6 will publish a booklet of short articles by people who attend the workshop, which will be widely distributed free of charge. The booklet will be similar in form to the one on "Fitting Molecular Potential Energy Surfaces", published after an earlier Workshop in the series in 1993. Each participant will be requested to write a short review-style article (400 - 2000 words) outlining their recent work in the area of the workshop. It should be emphasised that the articles are *not* intended to be abstracts of the talks given at the workshop, but should be much more general. It is intended that the booklet should give an interested reader from rather outside the field a good introduction. The booklet will be edited electronically, in LaTeX, and *only* email submissions will be accepted. The deadline for receipt of contributions has been extended to 5 January 1998.

Organising committee: Jeremy M. Hutson Markus Meuwly, Andreas Ernesti Nicholas J. Wright  
Postal address: Mr. N. J. Wright, Department of Chemistry, University of Durham, Durham, DH1 3LE, England Tel. +44 191 374 3123 FAX +44 191 384 4737

## **2. International Symposium on "Molecular Science of Excited States and Nonadiabatic Transitions"**

Institute for Molecular Science, Okazaki, Japan, March 25 - 28, 1998.

The Institute for Molecular Science (IMS) has been recognized as a Center of Excellence (COE) officially by The Ministry of Education, Science, Sports, and Culture of Japan. By the financial support from The Ministry (limited, of course!) we have an opportunity to organize an international symposium within this Japanese fiscal year. Considering the recent remarkable theoretical progress in the basic theory of nonadiabatic transition, quantum chemistry of excited states, and various nonadiabatic dynamics, we have determined the title of the symposium as "Molecular Science of Excited States and Nonadiabatic Transitions". The symposium will be held from March 25(Wed.) through 28(Sat.) in 1998 at The Okazaki Conference Center. Nonadiabatic transition is a very interdisciplinary phenomenon and concept, making an important mechanism of state and/or phase change in various fields of physics, chemistry, and biology. Recent theoretical progress in the related various fields is remarkable, and we think that it is really timely and valuable to organize such a symposium to stimulate interdisciplinary information exchange and discussions and to promote further developments. We would like to cover the following subjects:(1) basic theory of nonadiabatic transition, (2) quantum chemistry of excited states, (3) nonadiabatic molecular processes in gas phase, condensed medium, and biology.

Program details will be provided at a later date. Those who are interested in, please contact Yoshitaka Tanimura or Hiroki Nakamura of Department of Theoretical Studies, IMS.  
e-mail:[tanimura@ims.ac.jp](mailto:tanimura@ims.ac.jp), [nakamura@ims.ac.jp](mailto:nakamura@ims.ac.jp), fax: 81-564-53-4660.

### **3. Faraday Division, Royal Society of Chemistry - Faraday Discussion no. 109 CHEMISTRY AND PHYSICS OF MOLECULES AND GRAINS IN SPACE**

The University of Nottingham, UK, 15-17 April 1998

The Final Programme, Application Form, Bursary and Registration details for this meeting are now available and can be obtained by

1) Mail or E-mail from Ms S Riaz (please see reply form below); 2) Visiting the Faraday Discussion 109

Website: <http://www.nottingham.ac.uk/faraday.html>

The Conference Application Form is now available in downloadable postscript formats from a link on the FD 109 web pages, or from <http://brian.chem.nott.ac.uk/form/form.html>

People who have already requested Conference Application (and Bursary Request) forms will receive these by post shortly.

### **4. XXIII INFORMAL CONFERENCE ON PHOTOCHEMISTRY Pasadena, California USA, May 10-14, 1998**

The conference will take place in Pasadena, California, approximately 8 miles northeast of downtown Los Angeles at the Pasadena Center. The Center is a modern conference facility conveniently located near hotels and restaurants. Excursions will be planned to nearby sites of interest including the NASA/Jet Propulsion Laboratory, the new Getty Center, and the Huntington Library and Gardens.

The conference registration fee will be US 225 (*students* :50) before April 1, 1998 and 275 (*students* :100) after. There will be a limited amount of travel support available for graduate students. Nearby hotels will be used to house conference attendees. Complete information regarding location and rates will be provided in the Second Circular and Call for Papers, to be distributed approximately Feb. 15, 1998. For further information about the scientific program, contact Dr. Stanley Sander Jet Propulsion Laboratory Tel: (818) 354-2625 Fax: (818) 393-5019 Email: [ssander@jpl.nasa.gov](mailto:ssander@jpl.nasa.gov)

Professor Mitchio Okumura California Institute of Technology Tel: (626) 395-6557 Fax: (626) 568-8824 Email: [mo@cco.caltech.edu](mailto:mo@cco.caltech.edu)

About conference arrangements, contact Conferences Administration Services M/S T-1200 Jet Propulsion Laboratory 4800 Oak Grove Drive Pasadena, CA 91109 Tel: (818) 354-5556 Fax: (818) 393-4992 Email: [conf.admin@jpl.nasa.gov](mailto:conf.admin@jpl.nasa.gov)

WEB SITE: <http://www.cco.caltech.edu/photons/>

### **5. 53rd OHIO STATE UNIVERSITY INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY**

June 15-19, 1998, Columbus, Ohio, USA

Executive committee: Terry A. Miller, Chair Frank C. DeLucia Eric Herbst C. Weldon Mathews Russell M. Pitzer

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

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

### **6. MOLECULAR PHYSICS AND CHEMICAL REACTION DYNAMICS: Fundamental aspects and application to atmospheric and environmental sciences**

Summer School June 16-25 1998, Jonkerbosch Conference Center, Nijmegen (The Netherlands)

Organizers: Françoise Masnou-Seeuws (Laboratoire Aim Cotton, Orsay, France), W. J. van der ZANDE (FOM Institute, Amsterdam, the Netherlands) and F. Vecchiocattivi (University of Perugia, Italy).

Lecturers who have already accepted to participate include: D. Bassi (Trento), D. Clary (London), T. Slinger (Menlo Park), K. Bergmann (Kaiserslautern), G. Le Bras (Toulouse), W.J. van der Zande (Amsterdam),

P.Builtjies (Utrecht), H.J. Loesch (Bielefeld), F. Vecchiocattivi (Perugia), P. Casavecchia (Perugia), A. Orr-Ewing (Bristol), A. M. Wodtke (Santa Barbara), D. Parker (Nijmegen).

Scientific Programme: Chemical reactive and photofragmentation processes will be treated from the molecular point of view, with the aim of providing information on the role of microscopic properties in determining the relationship between structure and chemical as well as photo-reactivity. Laboratory quantum state resolved experiments as well as semi- classical and quantal theory of state-to-state reactions will be lectured upon. Applications are abundantly found in atmospheric sciences: the complex ozone (photo)-chemistry and the ozone hole; the role of photodissociation in protecting the earth from of the UV radiations; the impact of cosmic rays on the composition and temperature of the earth atmosphere. A link will be made towards atmospheric science by discussing rate constant determination and the importance of large chemical-box models of the atmosphere.

Registration: The school is opened to 60 graduate students and post-doctoral young researchers, both theoretical and experimental, in the fields of reactive scattering, photofragmentation and the atmospheric sciences. The registration fee is Dfl 300. Lodging expenses of EC students or post-docs will be covered by grants from the TMR Program of the European Commission. Such grants are also available for students from Iceland, Liechtenstein, Norway or Israel. Limited financial support is available for students/post-doctoral fellows from non-EC countries in Central or Eastern Europe. A few students will be admitted from other parts of the world provided they pay for their staying expenses. Candidates are invited to contact the School Coordinator before May 1st: Louise Roos, FOM-Institute for Atomic and Molecular Physics (AMOLF), Kruislaan 407, 1098 SJ Amsterdam, The Netherlands, tel. +31 20 608 1234 - fax +31 20 668 4106, e-mail L.Roos@amolf.nl. More information at: <http://www.amolf.nl/SSSTMP/nijme-01.html>

## **7. FUNDAMENTAL ASPECTS OF SURFACE SCIENCE: ELEMENTARY PROCESSES IN SURFACE REACTIONS**

Acquafredda di Maratea, Italy, June 20-25, 1998

This conference incorporates the 4th European Conference on Gas-Surface Dynamics and the 3rd European Conference on Lasers in Surface Science. Chairman: Mats Persson (Göteborg), Vice Chairman: Christof Wöll (Bochum)

A central issue in surface science is the identification and description on an atomic level of elementary dynamical processes underlying various surface phenomena in nature. Some typical examples of such phenomena are heterogeneous catalysis, oxidation, friction and wear, and atmospheric reactions on ice surfaces. The study of such processes, which is the theme of this meeting, is now possible thanks to recent advances in our knowledge of the geometric and electronic structure of adsorbates on surfaces and to recent developments of experimental and theoretical approaches to study the dynamics at surfaces. Spectacular examples of these approaches, which also form the basis for this meeting, include on the experimental side state-resolved molecular beam experiments, atomic and molecular manipulation by scanning tunneling microscope, femtosecond laser techniques, and on the theoretical side the developments of reliable total energy calculational schemes based on density functional theory and classical and quantum molecular dynamics calculations.

The meeting will have sessions of talks on: Gas-surface scattering; Reaction dynamics; Photo dynamics and chemistry; Potential energy surfaces; Chemistry on the nanoscale; Cluster deposition, growth and diffusion; Surface reactions and catalysis; New frontiers. Time will be available for presentations to be selected from the participant's abstracts. Poster sessions will be included to which all participants may contribute. There will be a special prize for the best student poster presentation. Applications from young investigators are encouraged and funds are available to subsidize the selected applicants.

Invited speakers who have already accepted to participate include:

Flemming BESENBACHER, Aarhus, Denmark; Wendy BROWN, Cambridge, UK; George DARLING, Liverpool, UK; Gerald DUJARDIN, Orsay, France; Riccardo FERRANDO, Genova, Italy; Jürgen HAFNER,

Wien, Austria; Ulrich HÖFER, Garching, Germany; Klaus KERN, Lausanne, Switzerland; Antonello De MARTINO, Palaiseau, France; Gil NATHANSON, Madison, USA; Hrvoje PETEK, Saitama, Japan; Bene POELSEMA, Enshede, Netherlands; Greg SITZ, Austin, USA; Adolf WINKLER, Graz, Austria; Joost WINTTERLIN, Berlin, Germany; Martin WOLF, Berlin, Germany; Igor ZORIC, Göteborg, Sweden  
DEADLINE FOR APPLICATION AND ABSTRACTS: MARCH 23, 1998

More details is available at the website of the European Research Network on Dynamics of Gas-Surface Interactions:

<http://www.fhi-berlin.mpg.de/gsd/ED4.html>

and at the ESF website

<http://www.esf.org/euresco/pc96.htm>

and in paper form by direct enquiry to our Conference officer below.

Application form is available in electronic form through the ESF website at

<http://www.esf.org/db/eurescoaf.idc?> and in paper by enquiry to Anne Hermans, 1 Quai Lezay Marnesia, 67800 Strasbourg Cedex, Fax: (0033) 3 88 36 69 87, Email: [Euresco@esf.org](mailto:Euresco@esf.org)

## **8. CCP6 WORKSHOP ON QUANTUM STATES OF MOLECULES AT DISSOCIATION**

University College London, 28-30 June 1998

The workshop covers aspects of molecular quantum states at the dissociation limit and will be held as a satellite meeting to the Faraday Discussion No: 110 on Chemical Reaction Theory at University of St Andrews on 1-3 July 1998. The study of vibrational states and resonances in molecules near dissociation provides an important link between high resolution spectroscopy and reaction dynamics. Recently, there have been a number of exciting developments in the theory of these states and many of these will be reviewed at the workshop.

The workshop will be held on 28-30 June 1998 at University College London and is sponsored by CCP6, the EPSRC Collaborative Computational Project on Heavy Particle Dynamics. It will consist of 6 invited talks and a number of shorter oral presentations. Sessions will commence at 9am Monday, 29 June 1998 and the workshop will end at lunchtime on Tuesday, 30 June 1998. Participants will be accommodated in Ramsay Hall and the Scientific Sessions will be held in the Chemistry Department Lecture Theatre.

INVITED SPEAKERS: W.H. Miller, University of California, USA; D.G. Truhlar, University of Minnesota, USA; J.M. Bowman, Emory University, USA; H.S. Taylor, University of Southern California, USA; J.Z.H. Zhang, New York University, USA; A. Carrington, University of Southampton, UK;

FURTHER INFORMATION & REGISTRATION: URL: [www.tampa.phys.ucl.ac.uk/mqsd](http://www.tampa.phys.ucl.ac.uk/mqsd)

CONTACT ADDRESS: CCP6 Workshop, c/o Prof. J. Tennyson, Department of Physics & Astronomy, University College London, Gower Street, London WC1E 6BT, UK

Email: [j.tennyson@ucl.ac.uk](mailto:j.tennyson@ucl.ac.uk), Tel : +(44) 171 380 7809, Fax : +(44) 171 380 7145

ORGANISING COMMITTEE: D.C. CLARY, Department of Chemistry, UCL; J. TENNYSON, Department of Physics & Astronomy, UCL; R. PROSMITI, Department of Physics & Astronomy, UCL

## **9. The 1998 Gordon Research Conference on ATOMIC AND MOLECULAR INTERACTIONS**

Conference Chair: Bob Wyatt ([wyatt@quantum.cm.utexas.edu](mailto:wyatt@quantum.cm.utexas.edu)), Vice-Chair: David Chandler ([chandler@ca.sandia.gov](mailto:chandler@ca.sandia.gov))

The 1998 Gordon Research Conference on Atomic and Molecular Interactions will be held June 28-July 3, at Colby-Sawyer College in New London, New Hampshire.

For additional information, see the GRC web site:

<http://www.grc.uri.edu>

Application for the conference may be made in the following ways:

1. use the GRC web site given above (this is the easiest way!)

2. by email to: app@grcmail.grc.uri.edu

3. by snail mail, write to: Gordon Research Conferences, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892-0984 USA Please register early!!

### **10. Faraday Division, Royal Society of Chemistry - Faraday Discussion 110 " CHEMICAL REACTION THEORY" University of St Andrews, Scotland, 1-3 July 1998**

#### **CALL FOR ABSTRACTS**

This will be the first Faraday Discussion devoted purely to the theory of chemical reactions, one of the most rapidly developing areas of theoretical chemistry. Predictions on the dynamics of the reactions of small molecules can now be as reliable as experimental measurements and the accuracy of calculations on more complicated problems ranging from reactions of organic molecules to reactions on surfaces and in solution is improving at a very fast pace.

The committee specially welcomes theoretical or computational papers in the following areas:

- \* ab initio calculation of accurate potential energy surfaces for chemical reactions
- \* scattering theory for the accurate treatment of the reactions of small molecules
- \* extension of theory to dynamics and kinetics of larger molecules
- \* reactions of molecules on solid surfaces and in solution.

The papers chosen for the Discussion will be concerned with theory or calculations that can be tested by comparison with experiment. St Andrews University on the east coast of Scotland is over 500 years old and is a beautiful place to hold the meeting (especially in July). The accommodation facilities there are excellent. There are good connections to St Andrews from the international airport at Glasgow and also from Edinburgh. Contributions are invited for consideration by the Organising Committee. Titles and abstracts of about 300 words should be submitted no later than 1 JUNE 1997 to Professor D C Clary, Department of Chemistry, University College London, London WC1H OAJ (email: d.c.clary@ucl.ac.uk). Full papers for publication in the Faraday General Discussion 110 volume will be required by February 1998. Organising Committee: D C Clary (Chairman), J N L Connor, I H Hillier, S Holloway, W C Mackrodt, D E Manolopoulos, M A Robb

### **11. Symposium on Elementary Chemical Processes**

Department of Chemistry of the University, Perugia, Italy, 10-13 July, 1998

An *International Symposium* will be held on the occasion of the 70th birthday of Professor Gian Gualberto Volpi. The local organizing committee includes the members of the Perugia Group (home page <http://www.chm.unipg.it/chmgen/mb/mb.html>)

The symposium will focus on modern progress on experimental techniques (molecular and ion beams, internal state-selection), theoretical approaches (quantum, approximate quantum, statistical treatments) and applications (models for combustion and atmospheric phenomena). Note that the symposium will take place immediately before the ECAMP VI Conference (the Sixth European Conference on Atomic and Molecular Physics) to be held in Siena from July 14th to 18th, 1998 (see below). Those who are interested to participate, and to present communications, are invited to e-mail [AQUILA@HERMES.CHM.UNIPG.IT](mailto:AQUILA@HERMES.CHM.UNIPG.IT) or fax 39-75-5855606.

### **12. The Second RACI Conference on Physical Chemistry (CPC'98)**

The University of Queensland (St Lucia Campus), Brisbane, Queensland, Australia, 11-16 July, 1998

The second RACI (Royal Australian Chemical Institute) Conference on Physical Chemistry (CPC'98) will be held in Brisbane at the St Lucia campus of the University of Queensland from 11th-16th July, 1998. This follows the highly-successful first Conference (ANU, January 1995), and like the earlier conference will seek to provide a broad coverage of contemporary research topics in Physical Chemistry. Conference accommodation will be available at St. John's College on the St. Lucia campus.

Confirmed plenary speakers for the conference are: K. Balasubramanian, Arizona State University, U.S.A.;

L. Butler, University of Chicago, U.S.A.; I.-C. Chen, National Tsing Hua University, Taiwan; M. Gruebele, University of Illinois, U.S.A.; N. Handy, University of Cambridge, U.K.; P. Houston, Cornell University, U.S.A.; W.C. Lineberger, University of Colorado, U.S.A.; K. Liu, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan.; N. Makri, University of Illinois, U.S.A.; D. Manolopoulos, Oxford University, U.K.; S. Okazaki, Tokyo Institute of Technology, Japan.; V. Vaida, University of Colorado, U.S.A.

Further details regarding registration and submission of abstracts will be distributed shortly. If you wish to receive conference information electronically, please send a message to the address:

"CPC98@chemistry.uq.edu.au". Any other queries will also be handled via this address.

Organizing committee: Dr Sean Smith (University of Queensland), Professor A. Haymet (University of Sydney) and Dr S. Kable (University of Sydney).

### **13. ECAMP VI - The Sixth European Conference on Atomic and Molecular Physics** Siena - Italy, 14-18 July, 1998

#### **FIRST ANNOUNCEMENT**

The Sixth European conference organized by the Atomic and Molecular Physics Division of the European Physical Society will be held in Siena (Italy) from 14th to 18th July, 1998.

Abstracts and accomodation reservations will be due by 1st March 1998.

All the correspondence should preferably be made by e-mail at the address ECAMP98@UNISI.IT

Scientific Secretariat: V. Biancalana, E. Mariotti fax:39-577-298297

Organizing Secretariat: fax:39-577-298134

Further information can be found at the Conference Web page:

<http://www.unisi.it/fisica/ecamp98/welcome.htm>

### **14. Molecular Beam Sessions within the 21st INTERNATIONAL SYMPOSIUM ON RAREFIED GAS DYNAMICS**

Université de Provence, Marseille, France July 26 - 31, 1998

We would like to take the opportunity of the forthcoming RGD Symposium to try to gather together again the MB people and the RGD people, as in the past decades. Information is available using the Web:

<http://www.cnrs-bellevue.fr/rgd>

Deadlines will be extended accordingly and further information will be available soon. E-mail:

[rgd@cnrs-bellevue.fr](mailto:rgd@cnrs-bellevue.fr)

### **15. 13th Canadian Symposium on Theoretical Chemistry**

The University of British Columbia Vancouver, Canada, August 2 - 7, 1998

Chairmen: Grenfell Patey (University of British Columbia), Tom Ziegler (University of Calgary).

Further information: Theoretical Chemistry Secretariat UBC Conference Centre 5961 Student Union

Boulevard Vancouver, BC, Canada V6T 2C9 Telephone: 1 (604) 822-1050 Facsimile: 1 (604) 822-1069

E-mail: [registration@brock.housing.ubc.ca](mailto:registration@brock.housing.ubc.ca) Website: <http://www.conferences.ubc.ca/theochem.htm>

Deadline for Abstracts June 1,1998.

### **16. ICAP 16** University of Windsor, August 3 - 7, 1998

The 16th International Conference on Atomic Physics (ICAP) will be held at the University of Windsor, August 3 - 7, 1998. The conference will feature an outstanding program of invited papers covering the properties of atoms and their interactions with light. Especially important are the remarkable advances in lasers and laser techniques for precision measurement, the cooling and trapping of atoms, atom optics, and the use of these techniques for both fundamental measurements and technological applications. The Conference will feature a special Nobel Symposium on Cooling and Trapping. There will also be poster sessions for contributed papers.

Registration will initially be open to all interested persons up to the early registration date of March 1, 1998. After that, registration will be subject to availability of space. Registration can now be done on-line, and further information obtained from the web site: <http://icap.cs.uwindsor.ca>

Alternatively, send a request for a hard copy of the registration form and other literature to [icap@uwindsor.ca](mailto:icap@uwindsor.ca).

Gordon Drake, Chair, ICAP Local Organizing Committee, Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4, CANADA.

### **17. PRAHA98, 15th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY** Prague, Czech Republic, August 30 - September 3, 1998

You should preregister before January 1, 1998.

#### INVITED SPEAKERS:

LINDA R. BROWN, Jet Propulsion Laboratory, Pasadena, California, U.S.A. Laboratory spectroscopy for planetary remote sensing. HANS BUERGER, Bergische Universitaet - GH Wuppertal, Wuppertal, Germany Detecting spectra of new molecules: synergism with theory. ALAN CARRINGTON, University of Southampton, Southampton, UK. Microwave spectroscopy at the dissociation limit. ROBERT F. CURL, Rice University, Houston, Texas, U.S.A. The fullerenes from the viewpoint of thirteen years. HAUKE HARDER, Universitaet Kiel, Kiel, Germany. Multiple fitting of perturbation-allowed rotational spectra of symmetric top molecules. MARTINA HAVENITH-NEWEN, Universitaet Bonn, Bonn, Germany. Infrared spectroscopy of van der Waals clusters. FRANCOIS HERLEMONT, Universite des Sciences et Technologies de Lille, Lille, France. High resolution spectroscopy with a tunable sideband CO<sub>2</sub> laser. BRIAN J. HOWARD, Oxford University, Oxford, UK High resolution spectroscopic studies of open-shell van der Waals complexes: a sensitive probe of molecular interactions. JAN MAKAREWICZ, Adam Mickiewicz University, Poznan, Poland Quantum mechanical and semiclassical description of ro-vibrational dynamics of floppy molecules. TAKESHI OKA, University of Chicago, Chicago, Illinois, U.S.A. High resolution infrared spectroscopy in molecular astrophysics: Observation of H<sub>3</sub><sup>+</sup> in various astronomical objects. TREVOR J. SEARS, Brookhaven National Laboratory, Upton, New York, U.S.A. Transient frequency modulation spectroscopy of molecular free radicals. MIKHAIL Yu. TRETYAKOV, Institute of Applied Physics, Russian Academy of Sciences, Nizhnii Novgorod, Russia. Spectroscopy in the terahertz region: new developments of experimental techniques.

The conference will be held in Prague-Troja [approx. 5 km north of Wenceslas Square and less than 1 km from the Metro (subway/underground) station Nadrazi Holesovice], in buildings of the Charles University. The local organization will be undertaken by the J. Heyrovsky Institute of Physical Chemistry in the Academy of Sciences of the Czech Republic, Prague. In 1998, the Charles University celebrates the 650th anniversary of its foundation on April 7th, 1348, and the PRAHA98 meeting will form part of this celebration.

Note also that the conference "EUCMOS XXIV: 24th European Congress on Molecular Spectroscopy" will take place in Prague August 23-28, 1998, that is during the week before PRAHA98. Further information is available from the World Wide Web at <http://staff.vscht.cz/eucmos/xxiv/>.

There will be 12 invited lectures. Contributions, which will be presented partly as posters and partly as contributed lectures, are invited in the fields of:

Observation, measurement, and analysis of high resolution rotational, vibrational, or electronic spectra of molecules (radicals, ions, complexes, clusters, ...) in the gas phase or in matrices.

Experimental techniques for observing such spectra. Theory assisting the prediction, simulation, and interpretation of them. Applications in related fields such as the physics and chemistry of the atmospheres of planets and cool stars, the physics and chemistry of the interstellar medium, chemical kinetics, etc.

Deadline for final registration and submission of abstracts: May 1st 1998.

Deadline for final reservation of accommodations: May 1st 1998

The conference has a home page on the World Wide Web with URL

<http://www.chem.uni-wuppertal.de/conference/>

ftp server: ——— The conference has an ftp server at  
[wcpj2.chemie.uni-wuppertal.de](http://wcpj2.chemie.uni-wuppertal.de) (132.195.9.35)

Use "ftp" or "anonymous" as user id and enter your complete e-mail address as password. The conference files are in the directory pub/praha98. The ASCII file read.me gives a list of the available files and describes their contents.

Preregistration: You should preregister (i.e., signal your intent to participate in the conference and/or request the second circular) before January 1st 1998. We would much prefer you to use the fill-out-form of our WWW home page for preregistration. This is not only convenient for you, it also represents by far the easiest way for us to process your data.

### **18. MOLEC XII Conference** Bristol, UK, 6-11 September 1998

Preliminary announcement

The 12th European Conference on Low Energy Molecular Collisions will be held in Bristol, UK, from 6 to 11 September 1998. Requests to be included in the conference mailing list may be made through the conference Web page (<http://www.tlchm.bris.ac.uk/molec/molec.htm>).

The Web page will be updated periodically as the program is finalised. Professor J.C. Polanyi has agreed to give a keynote lecture at the conference.

For further details contact Gabriel Balint-Kurti ([Gabriel.Balint-Kurti@Bristol.ac.uk](mailto:Gabriel.Balint-Kurti@Bristol.ac.uk)).

### **19. 15th International Symposium on Gas Kinetics** Bilbao, Spain, 6-10 September 1998.

Announcement of the keynote speakers are given in the mailed first circular and in the web page (<http://www.vc.ehu.es/gaskin98>)

Further details from Prof. F. Castano ([qfpcalf@lgdx02.lg.ehu.es](mailto:qfpcalf@lgdx02.lg.ehu.es)) or from the Gas Kinetics Group Secretary, Dr J.M.C. Plane, E-mail: [j.plane@uea.ac.uk](mailto:j.plane@uea.ac.uk)

The Secretary, 15th International Symposium on Gas Kinetics, Universidad del Pais Vasco, Departamento Quimica Fisica, Facultad de Ciencias, Apartado 644, E-48080 Bilbao, Spain, Fax: +34 (9)4 4648500, E-mail: [gaskin98@vc.ehu.es](mailto:gaskin98@vc.ehu.es)

### **20. THE SIXTH BRIJUNI CONFERENCE: END OF CENTURY STATE OF SCIENCE** Brijuni (Brioni) Island, Croatia, 7-11 September 1998

The VI-th conference on the island Brioni will cover the state of art of physics and chemistry (physical).

More detailed information about the topics covered, speakers and the site can be obtained at the web-site address <http://www.irb.hr/dbosanac> . Otherwise the information can also be obtained directly from S. Danko Bosanac at [DBOSANAC@FAUST.IRB.HR](mailto:DBOSANAC@FAUST.IRB.HR)

### **21. COMET XVI (XVI International Conference on Molecular Energy Transfer)**

Assisi, Italy, 20-25 June, 1999

Piergiorgio Casavecchia (Chair) and Antonio Laganà (Co-Chair).

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

A Web-page is being prepared at the URL address:

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

### **22. THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE**

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

James J. Valentini, Chair, 1999 Dynamics of Molecular Collisions Conference

## **d. Special announcement**

**A special issue of Journal of the Chemical Society Faraday Transactions on  
CHEMICAL REACTION THEORY will be published in 1999**

Contributions in the form of regular papers are invited by 31 October 1998 in the following areas:

- \* ab initio calculation of accurate potential energy surfaces for the chemical reactions.
- \* Scattering theory for the accurate treatment of small molecule reactions.
- \* Extensions of the theory for understanding the dynamics and kinetics of large molecules.
- \* reactions of molecules on solid surfaces.
- \* reactions of molecules in solution.

Further information from:

Professor J. N. L. Connor, Department of Chemistry,  
University of Manchester, Manchester M13 9PL, England.  
e-mail: J.N.L.Connor@Manchester.ac.uk