

# Molecular Dynamics News

number 95, June 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 has been accepted - otherwise state *unpublished*).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 96 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 (#95). The closing date for issue number 96 is August 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**

#### **ANNOUNCEMENT OF A FREE CHAIR**

Chair as a lecturer (associate professor) in physics at the Physics Department, Royal Institute of Technology (KTH), Stockholm, Sweden.

The chair is normally appointed for an initial period of three years followed by a permanent appointment without further application. The chair concerns 50 modern optics, non-linear optics or laser physics. The remaining 50 undergraduate teaching which is expected to be performed in Swedish when required. The applicant must have a PhD degree in physics and experience of university teaching. Equal weight is put on scientific and pedagogic skills. The applicant is expected to apply for external financing for his/her research. Individual salaries are applied at KTH. Please, give your salary request in the application.

More information concerning the chair is given by the Department Head, Prof. Per Carlson, ph. 46-8-161044, e-mail [carlson@msi.se](mailto:carlson@msi.se) and the professors Klaus Biedermann, ph. 46-8-790 7283, e-mail: [kb@optics.kth.se](mailto:kb@optics.kth.se), Ari Friberg, ph. 46-8-790 729; e-mail: [atf@optics.kth.se](mailto:atf@optics.kth.se) and Stig Stenholm, ph. 46-8-790 7269; e-mail: [stenholm@atom.kth.se](mailto:stenholm@atom.kth.se).

The applicant should include the following documents:

1. Curriculum vitae.
2. List of scientific publications documenting the competence.
3. Short description of scientific, pedagogic and administrative activities.
4. Ten publications ranked by the applicant as the best ones.

These items should be packed in three identical packages.

5. One copy of remaining publications in a separate package.

Most lecturers at KTH are male. KTH therefore welcomes applications from females. More information about the Department of Physics can be found at the www-address: <http://www.physics.kth.se> The application should be sent to Department of Physics, Royal Institute of Technology (KTH), SE 10044 Stockholm, Sweden and should arrive before 1998-06-25. Give the ref. number 510-99-98

Dr. Lars-Erik Berg, Atomic and Molecular Physics, Department of Physics, Royal Institute of Technology (KTH), SE-100 44 Stockholm, Sweden Phone +46 8 7907124, FAX +46 8 200430, e-mail: [berg@atom.kth.se](mailto:berg@atom.kth.se), <http://www.atom.kth.se/berg/lasres.html>

#### **ASSISTANT PROFESSOR, MEMORIAL UNIVERSITY OF NEWFOUNDLAND**

Applications are invited for a tenure-track position in the Department of Mathematics and Statistics at the Assistant Professor level, with primary research interest in Computational Applied Mathematics. This position will support a new interdisciplinary graduate programme in Computational Science within the Faculty of Science. Participating departments in this programme include Chemistry, Computer Science, Earth Sciences, Mathematics and Statistics, Physics and Physical Oceanography. A PhD and demonstrated ability to undertake interdisciplinary research and capacity to provide expert advice on topical problems in modern scientific computing are required.

This position will initially be supported by a Memorial University Research Infrastructure Funding in Targeted Areas grant. Startup research funding will also be available.

Applications marked REF:MS/CAMAT/98, with complete curriculum vitae, a research plan, a statement of present teaching interests, the names and e-mail addresses of at least three referees should be sent to: MS/CAMAT/98

Department of Mathematics and Statistics  
Memorial University of Newfoundland  
St. John's, Newfoundland, Canada  
A1C 5S7

Closing date for receipt of applications is July 15, 1998 or until the position is filled. Further details can be obtained from head@math.mun.ca. This position is subject to final budgetary approval.

Memorial University is committed to the principle of equity in employment. In accordance with Canadian Immigration requirements, priority will be given to Canadian citizens and permanent residents of Canada.

### **DEPARTMENT HEAD, MAX-BORN-INSTITUT FOR NONLINEAR OPTICS AND SHORT PULSE SPECTROSCOPY**

This position is expected to begin as early as 1 July 1998, and the candidate is expected to have a high level of competence and scientific creativity in conducting and further developing the interdisciplinary research program. Ability to motivate and guide a research team of presently 25 scientists, research students and technical staff is necessary, as well as evidence that the candidate can provide successful research leadership in an interdisciplinary environment involving other departments of the institute. The salary level for this high level of responsibilities is equivalent to that of a C3 professor in an German university. We expect an active engagement in academic teaching at one of the universities in Berlin or Brandenburg, in attracting external users from academia and industry for co-operative projects using the MBI facilities. The successful candidate is also expected to acquire additional research funding from outside sources.

Requirements: Ideal candidates would be young experimental physicists or physical chemists who have already achieved some international recognition in their field of research and who are familiar with academic teaching ( equivalent to the German 'habilitation'). They should have experience with laser spectroscopic methods and with at least one of the following research areas:

- surface physics/chemistry
- photophysics of large molecules, possibly including biomolecules
- ultrafast physics
- experiments with synchrotron radiation

Applications should be sent to Prof. I.V. Hertel, Director Division A, Max-Born-Institut, Rudower Chaussee 6, D-12489 Berlin, Germany. The applications should include a CV, research plan, summary of accomplishments since the PhD, and a list of professional references.

Tel: (030) 6392-1200, FAX: (030) 6392-1209, e-mail: hertel@mbi-berlin.de

## **POST DOCTORAL AND VISITING**

### **EXPERIMENTALIST (POSTDOC OR YOUNG SCIENTIST) POSITION AT INLN, CNRS, NICE, FRANCE.**

An experiment: we look on platinum wire put into a gas flow, and register hot spots and waves initiated by a laser beam. The challenge is to understand mechanisms of huge losses of noble metal in catalysis, and ways to diminish them. This is closely related to surface science also. Physico- chemical background is helpful but not obligatory. A curious and handy physicist who likes experiment will be successful here.

The position is till September 1999, it will start September 1998, although earlier starting date is negotiable too. The salary is 21 kF a month, for a European PostDoc (not from France: programme Training and Mobility of Researchers), and for a young scientist without PhD - depending on qualification. The fellowship is funded by the EU network "Nonlinear dynamics of spatially extended systems" and is intended for a citizen of a Member State of the European Community or of an Associated State.

Contact:

Prof. Valentin KRINSKY, Institut Non-Lineaire de Nice, U.M.R. C.N.R.S. 6618, Sophia Antipolis, 1361, Route des Lucioles, F-06560 Valbonne, FRANCE

E-mail krinsky@inln.cnrs.fr, Tel: ++33- 4-92-96-73-45, Fax: ++33- 4-93-65-25-17

### **POSTDOCTORAL POSITION**

### Atmospheric Photochemistry and Chemical Reaction Dynamics

A postdoctoral position in experimental chemical physics is available beginning June 1, 1998 with Simon North in the Department of Chemistry at Texas A&M University. The successful candidate will participate in experiments examining vector and scalar correlations in molecular fragmentation using frequency-modulated Doppler spectroscopy, resonance-enhanced multiphoton ionization time-of-flight, and laser-induced fluorescence. The research will focus on the photochemistry of atmospherically relevant molecules and the dissociation dynamics of small free radicals. Additional information can be found on the following homepage (<http://www.chem.tamu.edu/north/home.html>). A Ph.D. in chemical physics, physical chemistry, or physics is required. Preference will be given to candidates who have experience with pulsed and cw lasers, molecular beams, spectroscopy, and vacuum techniques. The position is initially for one year but may be extended for an additional year by mutual consent. The salary is negotiable. Interested candidates should send a cover letter, a curriculum vitae, and have three letters of recommendation sent directly from the referees to:

Prof. Simon W. North, Department of Chemistry, Texas A&M University, P.O. Box 300012, College Station, TX 77842

e-mail: [north@chemvx.tamu.edu](mailto:north@chemvx.tamu.edu), office: (409)-845-4947, Fax: (409)-845-2971

### **POSTDOCTORAL FELLOWSHIP, Institute of Physical Chemistry University of Zurich, Switzerland.**

A postdoctoral fellowship is available as of the 1st June or after in the group of Prof. J.R. Huber to work on one of the following projects: (1) photodissociation processes in molecules and molecular clusters (2) time resolved laser spectroscopy of molecules using the quantum beat method (3) liquid surface photochemistry in high vacuum. The first topic is studied using on a recently constructed REMPI-TOF flight apparatus and particular points of interest include the detailed investigation of energy partitioning and vector correlations in photodissociation processes and the study of cluster specific photochemistry. In the second field a pulsed dye amplifier generates Fourier transform limited nanosecond laser pulses which are then used to investigate intramolecular dynamics and electronic structure in molecules with a particular emphasis on transient species. The third project concerns the analysis of photoproducts ejected from a liquid surface after laser irradiation, using photofragment translational spectroscopy. The successful applicant should have a background in laser spectroscopy. Experience with molecular beam methods, the REMPI technique and/or time resolved spectroscopy would be of advantage.

Further information is available from:

World Wide Web: <http://www.unizh.ch/pci/huber.html>

Prof. J.R. Huber, PCI, Universitat Zurich, Winterthurerstr. 190, CH-8057 Zurich, Switzerland.

E-mail: [huber@pci.unizh.ch](mailto:huber@pci.unizh.ch), Tel: +41 1 635 4461, Fax: +41 1 635 6813

### **POSTDOCTORAL POSITION, UNIVERSITY OF BORDEAUX, FRANCE**

Applications are invited for a postdoctoral position, available immediately at the "Laboratoire de Physico-Chimie Moléculaire" of the "Université Bordeaux I", France. The successful candidate will be working with Dr. Michel Costes and Prof. Christian Naulin on neutral-neutral reactions that might be important in the chemistry of interstellar clouds. Experiments will be conducted on a recently developed crossed-molecular beam apparatus, which allows for scanning the relative translational energy of reactants down to values relevant to the conditions of the interstellar medium. Detection of products will involve vuv laser techniques. The project is funded by the European Commission under the TMR Network "Astrophysical Chemistry" program. Applicants must be European Union nationals (excluding France but including Associate States) and up to 35 years old. The duration of the fellowship is for 12 months. Net salary will be around 12000 FF/month. Applicants with a good background in gas-phase physical-chemistry and/or laser spectroscopy should submit a CV and the names of two referees to Dr. Michel Costes, UMR

5803 CNRS- Universite Bordeaux I, Laboratoire de Physico-Chimie Moleculaire, Universite Bordeaux I, 33405 Talence cedex, France. E-mail: costes@cribx1.u-bordeaux.fr.

**UNIVERSITE DE LAUSANNE, SWITZERLAND: POSTDOCTORAL POSITION, AVAILABLE AUTUMN 1998**

A postdoctoral position in Experimental Physics is available with Professor Majed Chergui at the Institut de Physique Experimentale, Universite de Lausanne, Switzerland. The exact starting date is negotiable. There are several available projects in the laboratory, which is equipped with an OPO nsec laser system and two femtosecond laser systems (one optimized for  $\sim$  50fs pulses). Possible projects include spectroscopic and real-time studies of Rydberg wavepackets, photochemistry of molecules in solutions or embedded in inert gas solids and light-induced deformations in solids. We also envisage to develop new detection schemes for condensed phase systems in relation to the nanosecond and/or the femtosecond experiments. The candidate will have to do some teaching and knowledge of french is desirable, but not a condition. In addition, he/she has the possibility to prepare for the equivalent of a habilitation. A PhD in physics or chemical physics is required. Experience with femtosecond and/or nanosecond lasers is highly desirable. The initial appointment will be for one year, but an extension of one or more years is possible. Interested applicants should send a resume and arrange to have two letters of reference sent to:

Prof. Majed CHERGUI, Institut de Physique Experimentale, Faculte des Sciences, BSP, Universite de Lausanne, Ch-1015 Lausanne, Switzerland

Further information is available through:

tel.: (21) 692 3660 (secr.), Fax.: (21) 692 3635 or 3605, email: Majed.Chergui@ipe.unil.ch,  
<http://www.unil.ch/ipe/>

**POSTDOCTORAL POSITION IN ATMOSPHERIC CHEMISTRY AT THE UNIVERSITY OF LEEDS**

Postdoctoral research associate position available to work within the atmospheric field monitoring group on a project involving a field instrument (FAGE) for the detection of OH and HO<sub>2</sub> radicals in the troposphere using laser-induced fluorescence. The appointment is for up to 2 years, starting as soon as convenient. The project will involve collaborative field work, instrument development (including the detection of other small radicals in the atmosphere by LIF) and the use of FAGE to study other applications in chemical kinetics and dynamics. Candidates must have a PhD in a relevant discipline (e.g. Physical Chemistry, Chemical Physics or Physics) and experience in the use of laser systems is highly desirable. Further information is available from Dr. Dwayne Heard, Tel. + 44 (0) 113 233 6471; fax +44 (0) 113 233 6565; email [dwayneh@chem.leeds.ac.uk](mailto:dwayneh@chem.leeds.ac.uk) and the following web sites:

<http://www.chem.leeds.ac.uk/Atmospheric/Field/fage/fage.html>

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

Interested applicants should send a detailed curriculum vitae, together with the names, phone numbers and e-mail addresses of two referees, to Dr. D. E. Heard, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK, and arrange for their two referees to send supporting letters of recommendation (email preferred).

**UNIVERSITY OF CALIFORNIA, SANTA CRUZ, Department of Chemistry**

Two postdoctoral positions for one or two years are expected to be available in July 1998 in the research group of Roger W. Anderson. The research will explore the optical, electronic properties, and growth of nanocrystalline silicon materials. Applicants should have a Ph.D. in physical chemistry, physics, or material sciences and they should have experience with at least one of the following: laser spectroscopy, fluorescence spectroscopy, photochemistry, thinfilm characterization, kinetics of crystal growth, molecular dynamics of solid phase growth, and electronic structure and related condensed matter physics of semiconductors.

Applicants should send a curriculum vitae, a summary of research experience, and arrange for two or three letters of recommendation to be sent to: Professor Roger W. Anderson, Department of Chemistry, University

of California, Santa Cruz, California 95064, USA. Telephone: (408) 459-2854, FAX: (408) 459-2935, E-mail: anderso@cats.ucsc.edu. Applicants should indicate their interest by electronic mail or FAX followed by a letter with application materials.

#### **POSTDOCTORAL POSITIONS, MAX-BORN-INSTITUT, BERLIN**

These positions are scheduled to start on 1 January 1999, and they are initially limited to a two year appointment at the salary level BAT IIa. Later an extension to a maximum of 5 years is possible if a habilitation can be experted within this time.

The succwssful candidates will have to carry out research in photophysics and photochemistry of thin films and adsorbates. This involves the use of ultrashort lasers as well as combined experiments with laser- and synchrotron-radiation at the MBI BESSY II beamline. The focus of the work will be on a) building up and using the latter facility in cooperation with external users and b) experiments studying ultrafast processes on free and adsorbed clusters and molecular systems using femtosecond laser sources. Participation in academic teaching is desirable.

Requirements: PhD in physics or physical chemistry or corresponding qualification as well as experience in one of the areas given above. Reserarch experience outside Germany is desirable.

Applications should be sent to Prof. I.V. Hertel, Director Division A, Max-Born-Institut, Rudower Chaussee 6, D-12489 Berlin, Germany. The applications should include a Vita and lists of publications and references. Tel: (030) 6392-1200, FAX: (030) 6392-1209, e-mail: hertel@mbi-berlin.de

#### **UNIVERSITY OF MELBOURNE, School of Chemistry**

Applications are invited for a post-doctoral position in the area of spectroscopy of gas phase cluster ions and radicals, within the group of Dr. E.J. Bieske, at The School of Chemistry, The University of Melbourne, Australia. The laboratory is well equipped with Nd:YAG pumped dye laser and optical parametric oscillator systems, a cavity ring down spectrometer, and a tandem mass spectrometer. The appointment is for between two and three years, to start immediately. Applicants should have a background in laser spectroscopy or mass spectrometry. The salary range is A40,606 – A43,588 (A= 0.67US). Applications should include the names and email or fax adresses of two referees.

Enquires (preferably email in the first instance) and applications should be directed to:

Dr. Evan Bieske, School of Chemistry, The University of Melbourne, Parkville, Victoria 3052, Australia  
email: e.bieske@chemistry.unimelb.edu.au, Ph: ++61 3 9344 7082, Fax: ++61 3 9347 5180

#### **INSTITUTE OF ELECTRONIC STRUCTURE, HERAKLION-CRETE**

A postdoctoral position (renewable for up to 36 months) at the Institute of Electronic Structure and Laser in Heraklion-Crete (Greece) is available starting in April 1998. The position is part of the IMAGINE Project recently funded by the European Commission under the TMR programme, and involves six laboratories: FOM (The Netherlands), Universitat Bielefeld (Germany), University of Bristol (UK), FORTH(Greece), 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).

IMPORTANT!!! 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.

Research areas of interest in our laboratory at IESL-FORTH include

1. Photofragmentation studies of halogen containing species ( $\text{Cl}_2$ ,  $\text{CH}_3\text{Br}$ ,  $\text{CH}_3\text{I}$ )
2. Multiphoton Dissociation of molecules ( $\text{CS}_2$ ,  $\text{NO}_2$ ,  $\text{CH}_3\text{I}$ )
3. Photofragment/photoelectron imaging using short pulse (fs-ps)lasers.

4. Negative ion photodetachment spectroscopy via e- imaging.
5. Ion-molecule reactive scattering experiments.

List recent publications: 1. PHOTOFRAGMENTATION STUDY OF  $\text{Cl}_2$  USING ION IMAGING, P.C. Samartzis, I. Sakellariou, T. Gougousi, T.N. Kitsopoulos, J. Chem. Phys. 107, 43 (1997)

2. TWO-PHOTON DISSOCIATION STUDY OF  $\text{CS}_2$  USING ION IMAGING, P.C. Samartzis and T.N. Kitsopoulos, J. Phys.Chem. 101, 5620 (1997).

3. PHOTOFRAGMENTATION OF  $\text{Cl}_2$  AT 308 NM, P.C. Samartzis, T. Gougousi, and T.N. Kitsopoulos, Laser Chem. 100, 1 (1998).

4. PHOTODISSOCIATION STUDY OF  $\text{CH}_3\text{Br}$  IN THE FIRST CONTINUUM, T. Gougousi, P.C. Samartzis and T.N. Kitsopoulos, J. Chem. Phys. 108, (1998).

Operating at FORTH is an Ultraviolet Laser Facility and detailed information concerning the available resources can be found at <http://www.iesl.forth.gr/ulf/>

Information concerning the largest Greek Island of Crete can be found at <http://www.interkriti.org/>

Candidates interested should send a CV to the address below or via email to: [theo@esperia.iesl.forth.gr](mailto:theo@esperia.iesl.forth.gr)

Theofanis Kitsopoulos, Asst. Prof. of Chemistry, Department of Chemistry, University of Crete and Institute of Electronic Structure and Laser (IESL-FORTH), P.O. Box 1527, 711 10 Heraklion-Crete, GR

tel: ++30-81-391467, fax: 391318

### **DUQUESNE UNIVERSITY, PITTSBURGH, Department of Chemistry**

A postdoctoral position is available in theoretical chemistry: a background in classical and mixed quantum-classical MD simulations is desirable. The initial appointment will be for one year, but funds are available for support beyond the first year.

The research project involves the investigation of electronic localization and conduction behaviors at metal-dielectric interfaces. These are systems where microscopically detailed experimental investigations are currently being pursued. A molecularly detailed theory to describe the electronic conduction-insulation behavior of metal-dielectric interfaces will be developed in close coordination with experimental results. There is also the possibility of collaborating in developing quantum mechanical instantaneous normal mode (INM) theories of liquid state spectroscopy.

The department of chemistry at Duquesne University is a very active theoretical environment with three theorists (including Dr. Jeffry Madura and Dr. Julian Talbot). Our interactions include joint weekly group meetings and formal and informal collaborations at all levels.

Relevant publications include:

Ferrel Bowen and Brian Space, "The Effective Mass of Excess Electrons in Condensed Xenon: Toward Methods for Modeling Metal-Dielectric Interfaces", J. Chem. Phys., 1997, v.107, p. 1922

Preston Moore and Brian Space, "An Instantaneous Normal Mode Theory of Condensed Phase Absorption: The Collision-Induced Absorption Spectra of Liquid  $\text{CO}_2$ ", J. Chem. Phys., 1997, v. 107, p.5635

Our web page: <http://nexus.chemistry.duq.edu/snes/chemistry/faculty/space.html>

To apply, send (email preferred) CV and at least 2 supporting letters to: Professor Brian Space, Duquesne University, Department of Chemistry, Pittsburgh, PA 15282-1530

For more information, please feel free to contact me at: email: [space@space1.chemistry.duq.edu](mailto:space@space1.chemistry.duq.edu), phone: (412)396-4732, or by FAX: (412)396-5683

### **UNIVERSITY OF CAMBRIDGE, Department of Chemistry**

Postdoctoral in Chemical Mapping of Cell and Virus Surfaces via Scanning Near Field Optical Microscopy  
Scanning near field optical microscopy (SNOM) gives images with a resolution less than the wavelength of light by scanning a sharpened optical fibre probe over a surface. By working in the near field the resolution is only limited by the size of the near field probe and resolution of between 10 - 80 nm can be obtained. We have constructed a unique reflection mode SNOM (Rev.Sci.Instrum 68,1448,1997) capable of working in

liquids and studying hydrated biological specimens, and have shown recently that it is possible to identify the position of monoclonal antibodies upon a virus surface. We are seeking a suitably qualified person to extend these studies and make considerable modifications to the instrument in order to improve its resolution and efficiency. The ultimate aim of the project is to map binding sites on virus and cell surfaces using fluorescently labelled antibodies.

A postdoctoral position for up to three years is available in the research groups of Dr David Klenerman and Dr Trevor Rayment in the Department of Chemistry, Cambridge University, to begin as soon as possible. Applicants should have a strong experimental background with experience in optics, laser spectroscopy or scanning probe methods. A background in molecular biology is not required since we collaborate with groups at the Laboratory of Molecular Biology, MRC Cambridge, and the Nuffield Department of Clinical Medicine Oxford, who will supply the samples used in these experiments however it is important that the person appointed is keen to learn about this area.

For further details please contact:

Dr. Trevor Rayment, Department of Chemistry, University of Cambridge, Lensfield Road, CAMBRIDGE CB2 1EW

Tel: 01223 336469, email: tr22@cus.cam.ac.uk

#### **UNIVERSITY OF HELSINKI, Laboratory of Physical Chemistry**

A postdoctoral position is available in the Laboratory of Physical Chemistry for one year. The monthly grant is about 2000 ECU (approx. 2175 USD) tax-free. The successful candidate who must be below 35 years old and who must of EU nationality (but not from Finland) is expected to perform theoretical and computational research in the field of overtone spectroscopy: local modes, Fermi resonances and potential energy surfaces. For recent publications from the Helsinki group see J. Chem. Phys. 101, 8380 (1994); 102, 3911 (1995); 102, 3945 (1995); 102, 5200 (1995); 103, 6861 (1995); 103, 6586 (1995); 104, 488 (1996); 106, 831 (1997); 106, 7931 (1997); 107, 1680 (1997). The Helsinki molecular spectroscopy group does both theoretical and experiment work and it consists of about 10 people. More information can be obtained from Prof. Lauri Halonen, tel. +358-9-19140280, fax +358-9-19140279, email lauri.halonen@csc.fi, <http://fkmarilyn.pc.helsinki.fi/>.

Please send the applications to the address: Prof. Lauri Halonen, Laboratory of Physical Chemistry, P. O. Box 55 (A. I. Virtasen aukio 1), FIN-00014 University of Helsinki, Finland. The closing date is 20th March 1998.

#### **UNIVERSITY COLLEGE LONDON, Theoretical/Computational Chemistry**

**\*\*Improved understanding of interactions in molecular solids, complexes and proteins through anisotropic atomic charge distributions\*\***

Zeneca Strategic Research Fund are funding a three year postdoctoral research position for fundamental research into intermolecular interactions. The research will lead to the quantification of model anisotropic atom-atom model potentials using ab initio molecular charge distributions, and their use in studying molecular recognition and crystal structure prediction. The project requires a recently (or nearly) qualified PhD in theoretical/computational chemistry with experience in molecular modelling or ab initio calculations. For further information, please contact Dr Sally Price (s.l.price@ucl.ac.uk, or Centre for Theoretical and Computational Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, 0171-504-4622), preferably before March 18th.

Dr S L Price (Dr S Price will be confused with Dr S D Price at same address) Centre of Theoretical and Computational Chemistry Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ

Phone: 0171 504 4622, Fax: 0171 380 7463

#### **OKLAHOMA STATE UNIVERSITY, STILLWATER, Department of Chemistry**

Postdoctoral Position Available: Theoretical/Computational Dynamics Studies of Many-Atom Systems. Experience in molecular modeling, classical dynamics, and Monte Carlo is desired. The research may involve formulating PESs, theoretical studies of unimolecular reactions of large molecules, predictions of crystal structures, and simulations of processes in molecular crystals. The appointment will be for one year, but renewable depending on funds and by mutual agreement. Interested candidates should contact (before May 1, 1998): Professor Donald L. Thompson, Department of Chemistry, Oklahoma State University, Stillwater, OK 74078. Phone: (405) 744-5174. FAX: (405) 744-6007. Email: dlt@osuunx.ucc.okstate.edu.

#### **UNIVERSITY OF NIJMEGEN, Department of Physics**

A postdoctoral position (renewable for up to 24 months) at the University of Nijmegen, Department of Molecular and Laser Physics is available starting in April 1998. The position is part of the IMAGINE Project recently funded by the European Commission under the TMR programme, and involves six laboratories: FOM (The Netherlands), Universitat Bielefeld (Germany), University of Bristol (UK), FORTH(Greece), 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 David Parker (Nijmegen).

IMPORTANT!!! 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.

Research areas of interest in our laboratory at Nijmegen include:

1. Photophysics of molecules relevant in atmospheric processes
2. Photofragment / photoelectron velocity map imaging
3. Crossed beam inelastic and reactive scattering experiments

List of recent publications:

1. Velocity map imaging of ions and electrons using electrostatic lenses: application in photoelectron and photofragment ion imaging of molecular oxygen. A.T.J.B. Eppink and D.H. Parker, Rev. Sci. Instrum. 68, 3477 (1997).
2. Photoelectron and photofragment velocity map imaging of state-selected molecular oxygen dissociation/ionization dynamics. D.H. Parker and A.T.J.B. Eppink, J. Chem. Phys. 107, 2357 (1997).
3. Production of maximally aligned O(<sup>1</sup>D) atoms from two-step photodissociation of molecular oxygen. A.T.J.B. Eppink, D.H. Parker, M.H.M. Janssen, B.Buijsse, and W.J. van der Zande, J. Chem. Phys. 108, 1305 (1998).
4. The sequential two photon dissociation of NO as a source of aligned N(<sup>2</sup>D), N(<sup>4</sup>S), and O(<sup>3</sup>P) atoms. B.L.G. Bakker, A.T.J.B. Eppink, D.H. Parker, M.L. Costen, G. Hancock, and G. Ritchie, Chem. Phys. Lett. 283, 319 (1998)

The department of Molecular and Laser Physics in Nijmegen consists of 40 senior and junior scientists specializing in fundamental and applied molecular physics. English is the most common language of our lab as a number of graduate students and postdocs are non-Dutch. More information on the department and the environs of Nijmegen can be found at:

<http://www.sci.kun.nl/mlf>

Candidates interested should send a CV via email to: [parker@sci.kun.nl](mailto:parker@sci.kun.nl) or to David H. Parker, Department of Molecule and Laser Physics, University of Nijmegen, Nijmegen, 6025ED, The Netherlands  
Tel. 31-24-3653423, Fax: 31-24-3653311

#### **LEIDEN UNIVERSITY, Leiden Institute of Chemistry**

A postdoctoral position is available for a joined theoretical chemistry and molecular astrophysics project of

the Leiden Institute of Chemistry and Leiden Observatory at Leiden University, The Netherlands in the group of Marc van Hemert and Ewine van Dishoeck. The position is financed for one year with the possibility of renewal for a second year, and can start anytime up to October 1998. The project involves the application of parallel computers in the quantumchemical and quantumdynamical description of photodissociation and rearrangement reactions of small molecules of astrophysical interest. A suitable candidate should i) be an expert programmer, ii) have ample experience with the techniques of parallel computing, like MPI and HPF, iii) have a good understanding of numerical mathematical physics methods, and iv) have a basic knowledge of quantumdynamics and quantumchemistry. The LIC has its own 15 node IBM SP computer and the group has ample access to the national supercomputer facilities.

Applicants should send a curriculum vitae, publication list and a brief statement of research interests, and arrange for at least two letters of recommendation to be sent before May 1 1998 to Dr. M.C. van Hemert, Leiden Institute of Chemistry, P.O. Box 9504, 2300 RA Leiden, The Netherlands (FAX: +31-71-5274488). Additional information can be obtained by e-mail through [marc@rulgle.leidenuniv.nl](mailto:marc@rulgle.leidenuniv.nl) or [ewine@strw.leidenuniv.nl](mailto:ewine@strw.leidenuniv.nl) (<http://strw.leidenuniv.nl>).

### **WEIZMANN INSTITUTE, REHOVOT, Department of Chemical Physics**

A position is available in the research group of David Tannor at the Weizmann Institute, with a flexible starting date. Applicants should have a strong background in theoretical chemistry or physics and numerical computations. Research possibilities include theoretical studies of

1) quantum and semiclassical studies of chemical reaction dynamics, (Chem. Phys. Lett. Chem. Phys. Lett. 262, 477 (1996); J. Chem. Soc. Faraday Trans. 93, 781 (1997).)

2) phase space approach to quantum condensed phase dynamics, (J. Chem. Phys. 107, 5236 (1997); *ibid.* 5141 (1997), J. Chem. Phys. in preparation).

3) laser cooling of molecular translational and internal degrees of freedom, (J. Chem. Phys. 99, 196 (1993); *ibid.* 106, 1435 (1997); J. Chem. Phys. in preparation).

4) Dynamics of multielectron atoms (J. Chem. Phys. in preparation).

The Weizmann Institute is a beautiful campus with a warm climate, with strong interactions among faculty members both on the campus and at other universities in Israel. The initial contract will be one year, renewable for a second year. Interested applicants should send a letter of interest outlining relevant experience, a brief CV and the names of three references to David Tannor at the address below.

Prof. David J. Tannor, Department of Chemical Physics, Weizmann Institute, Rehovot, Israel  
Phone:+972-8-934-2094, Fax:+972-9-934-4123

### **UNIVERSITY OF OXFORD, Physical and Theoretical Chemistry Laboratory**

Applications are invited for an EPSRC funded post-doctoral research assistantship in Reaction Stereodynamics, tenable for a period of 36 months, and to be held in the research group of Dr M. Brouard in the Physical and Theoretical Chemistry Laboratory, Oxford University. The research project concerns the experimental study of the stereodynamics of elementary gas phase reactions using polarized laser pump-probe techniques. Applicants should have experience in the use of pulsed laser systems, should be computer literate, and preferably have some background in the field of reaction dynamics. The post is available from 1 June 1998, or as soon after as possible, and the salary will be on the 1A scale at from 15,159 to 22,785 pounds sterling per annum.

Applicants should submit a curriculum vitae and arrange for two referees to write directly to Dr M Brouard, The Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ (email address [mark.brouard@chemistry.ox.ac.uk](mailto:mark.brouard@chemistry.ox.ac.uk)) by 1 May 1998. This post is open to non-UK nationals.

The University is an Equal Opportunities Employer.

### **UNIVERSITY OF NOTRE DAME, College of Science**

The University of Notre Dame seeks a Computing Associate for the College of Science. The incumbent will

be responsible for assisting and promoting effective computing in the College and facilitating the use of networked resources for teaching and research. The Computing Associate will understand the needs of each unit and encourage and support joint efforts among College units and other units on campus. An advanced degree, preferably in a science-related discipline, is required. The appointment will be at faculty rank (assistant professional specialist) for those with suitable academic background. For further information on the College of Science, see our web site at <http://www.science.nd.edu>.

Computing background should include broad experience in UNIX systems administration (SGI/IRIX, Sun/Solaris, and/or IBM/AIX) and familiarity with Windows/NT. Programming proficiency in FORTRAN, C or C++, and UNIX scripting languages is required. The candidate should be familiar with an assortment of scientific software, e.g., Mathematica, Biosym, and TeX. Experience with AFS, parallel programming, or multimedia is a plus. Experience in applying computer technology, preferably in an academic environment, is highly desirable.

The Computing Associate must have excellent interpersonal and communication skills, be able to work well in a collegial relationship with faculty and students, be flexible, and be highly motivated.

To be assured of maximum consideration, submit application consisting of a letter of application, resume, and names of three professional references to Professor Kathie Newman, Computing Associate Search, College of Science, University of Notre Dame, Notre Dame, IN 46556. Applications may also be sent by email to [newman.1@nd.edu](mailto:newman.1@nd.edu). Review of applications will begin immediately and will continue until the position is filled.

EOE/AA MINORITIES AND WOMEN ARE ENCOURAGED TO APPLY

### **UNIVERSITY OF GEORGIA, Department of Chemistry**

Photodissociation Spectroscopy and Dynamics in Mass-Selected Metal Ion Complexes

Weakly bound metal ion complexes ( $M^+ \cdot Rx$ , where  $M = Mg, Ca, Ti$ , etc. and  $R = Ar, CO_2, H_2O, N_2, C_2H_2$ , etc.) are investigated as models for metal cation solvation, metal-ligand bonding and metal ion atmospheric chemistry. Complexes are produced and cooled in a pulsed nozzle laser vaporization cluster source in a two-chamber molecular beam machine. The species produced are mass-analyzed and mass-selected with a reflectron time-of-flight mass spectrometer. Electronic states, vibrational frequencies and structures of these complexes are investigated with photodissociation spectroscopy. Complexes absorb near metal atomic transitions to populate bound excited molecular states, and then dissociation occurs following the absorption of one or more additional photons. New experiments use an infrared OPO to probe ligand-based vibrational overtones. These experiments determine the structure of metal ion complexes and their bond energies and follow the development of these properties as a function of cluster size. Instrumentation for this project includes the pulsed molecular beam machine with reflectron TOF mass spectrometer, a XeCl excimer laser for the cluster source (Lambda Physik EMG 101), an ArF excimer laser for photoionization (Lumonics PM-840), a YAG-pumped dye laser (Spectra-Physics GCR-170 with Lambda Physik ScanMate 2E and doubler unit) and a new YAG-pumped OPO/OPA system (Continuum 9010 YAG with "SunLite" OPO and doubler unit). Data collection with a digital oscilloscope (LeCroy 9410A) and laser scanning are controlled with a Pentium PC.

Recent Publications from this Project:

M.A. Duncan, "Spectroscopy of metal ion complexes: Gas phase models for solvation," *Ann. Rev. Phys. Chem.* 48, 63 (1997).

S.H. Pullins, J.E. Reddic, M.R. France and M.A. Duncan, "Photodissociation spectroscopy of  $Ca^+ \cdot N_2$ ," *J. Chem. Phys.* 108, 2725 (1998).

Michael A. Duncan, Department of Chemistry, University of Georgia, Athens, Georgia 30602  
phone: 706-542-1998, fax: 706-542-9454

### **MARQUETTE UNIVERSITY, MILWAUKEE, Department of Chemistry**

A post-doctoral position in experimental chemical physics is available with Scott Reid in the Department of Chemistry at Marquette University beginning June 1, 1998 (exact starting date is negotiable). The successful candidate will participate in experiments on the spectroscopy of jet-cooled radicals using a variety of experimental techniques including resonant four wave mixing, cavity ring down, and resonant photoionization spectroscopies. A Ph.D. in physical chemistry or chemical physics is required, and candidates having experience with nanosecond and picosecond Nd:YAG pumped dye lasers, pulsed molecular beams, and high vacuum equipment will be given preference. The salary is negotiable, and initial appointment will be for one year, with an extension of one or more years possible by mutual consent. Interested applicants should send (by May 15th) a curriculum vitae and have two letters of reference sent directly from the referees to:

Prof. Scott A. Reid, Department of Chemistry, Marquette University, P. O. Box 1881, Milwaukee, WI 53201-1881

email: Reids@vms.csd.mu.edu, Phone: (414) 288-7565/7715, FAX: (414) 288-7066

**UNIVERSITY OF PUERTO RICO, Department of Chemistry** A post-doctoral position is immediately available with Edwin Quinones in the Department of Chemistry at the University of Puerto Rico, Rio Piedras Campus. The successful candidate will carry out photofragmentation studies on weakly bound clusters. A Ph.D. in physical chemistry, chemical physics, or physics is required. Preference will be given to candidates with experience with nanosecond laser systems (Nd:YAG lasers, excimer-pumped dye lasers) and pulsed molecular beams. The position has a salary of \$28,000 (US dollars) per year, plus medical plan. Interested candidates should send a cover letter, a curriculum vitae, and arrange for three letters of reference to be sent directly from the referees to:

Edwin Quinones, Department of Chemistry, University of Puerto Rico, P.O. Box 23346 UPR Station, San Juan, Puerto Rico 00931-3346

fax (787) 759-6885, tel. (787) 764-0000 Ext. 4810

**UNIVERSITY OF ILLINOIS, CHICAGO, Department of Chemistry**

A post-doctoral position is open in the group of Prof. Robert Gordon at the University of Illinois at Chicago in the areas of coherent control and molecular optics. The research associate may work on either of two projects (or both!). The first project is a continuation of ongoing work described in recent publications in *Science* (270, 77 (1995)) and *Physical Review Letters* (79, 4108 (1997)), in which we demonstrated coherent phase control over the branching between ionization and dissociation of HI and DI. Future experiments will include bond-selective photochemistry and control over the angular distributions of photofragments. A recently completed photofragment imaging machine will be used for some of these experiments. In the second project a tightly focused laser beam will be used to create a "molecular lens" that is capable of focusing and steering a molecular beam. Possible experiments include using the focused molecular beam to create nanostructures on a surface and measurement of the alignment of pendular states using a femtosecond probe.

Candidates for this position should have experience with dye lasers, pulsed molecular beams, and ion optics. The position is to start in the Fall of 1998, and funding is available for more than one year. Please send resumes and arrange for letters of recommendation to be sent to Robert Gordon, Department of Chemistry (m/c 111), University of Illinois at Chicago, 845 W Taylor Street, Chicago, IL 60607-7061  
phone: (312)996-3280, fax: (312)996-0431

**UNIVERSITY OF PERUGIA, ITALY, Department of Chemistry**

A post-doctoral position will be available in the laboratory of Prof. P. Casavecchia, Department of Chemistry, University of Perugia, Italy, starting November 1998 or shortly afterwards (January 1999). The initial appointment is for one year, but funds are available for extension to a second year based upon mutual agreement. The position is funded by the European Commission within the TMR (Training and Research

Mobility) Research Network Program "ASTROPHYSICAL CHEMISTRY". This program involves eight laboratories : University of Birmingham (UK), University College London (UK), University of Göttingen (Germany), Technische Universität Chemnitz (Germany), University of Rennes (France), Observatoire de Paris, Meudon (France), University of Bordeaux (France), and the University of Perugia (Italy), with research groups headed by Ian Smith and Ian Sims (Birmingham), David Clary and David Williams (UCL), J. Troe (Göttingen), D. Gerlich (Chemnitz), B. Rowe (Rennes), E. Roueff (Meudon), M. Costes (Bordeaux), and P. Casavecchia (Perugia). All have excellent facilities and extensive research interests. **IMPORTANT !** 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, Liechtenstein, or Norway) to be eligible for this post-doc position. Furthermore, you may not be a national of the state of the laboratory to which you are applying. The focus in our laboratory is on studies of chemical reaction dynamics by 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 Astrophysical Chemistry will be pursued. The post-doc is also expected to spend up to one month each year in another laboratory of the TMR network. Recent selected publications from the group can be found in : J. Chem. Soc. Faraday Trans. (Faraday Research Article) 91 (1995) 575 ; Advanced Series in Physical Chemistry - Vol. 6: The Chemical Dynamics and Kinetics of Small Radicals, eds. K. Liu and A. Wagner (World Scientific, Singapore, 1995), cap. 9 ; Chem. Phys. 207 (1996) 389 ; Science 273, (1996) 1519 ; Molecules in Astrophysics: Probes and Processes, IAU 178 , ed. by E. F. van Dishoeck (Kluwer, Amsterdam, 1997), pp. 271-280 ; J. Phys. Chem. A, 10 1, (1997) 6455 ; J. Chem. Phys. 108, xxx (1998, 22 April issue, n. 16). Experience in vacuum technology, molecular beams and reaction dynamics is desirable. Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The names and addresses of two referees should also be provided at this time. Informal enquiries are also welcomed.

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto, 8 06123 Perugia, Italy. E-mail : piero@scatter.chm.unipg.it (Phone : (+39) (75) 585-5514 -Fax : (+39) (75) 585-5606).

## **b. Preprints**

**Femtosecond Transition State Spectroscopy of Solids: Electronic "Bubble" Formation in Solid H<sub>2</sub>**  
Chemical Physics Letters 279 (1997) 65

C. Jeannin, M. T. Portella-Oberli, F. Vigliotti and M. Chergui

Inst. de Physique Experimentale, Université de Lausanne, CH-1015 Lausanne, Switzerland

We report on the femtosecond dynamics of electronic bubble formation in solid H<sub>2</sub> following Rydberg state excitation of an NO impurity. The bubble is formed coherently by the collective displacement of the H<sub>2</sub> molecules in about 1.5 ps.

**The visible emission and absorption spectrum of C<sub>60</sub>**

J. Chem. Phys. 107 (1997) 8731

A. Sassara, G. Zerza, M. Chergui

Inst. de Physique Experimentale, Université de Lausanne, CH-1015 Lausanne, Switzerland

F. Negri and G. Orlandi

Dipartimento di Chimica, Univ. di Bologna, Bologna, Italy

The fluorescence and fluorescence-excitation spectrum of C<sub>60</sub> in Ne and Ar matrices is discussed in relation to new calculations of the oscillator strengths of Jahn-Teller and Herzberg-Teller induced transitions.

**Rydberg states in quantum crystals: NO in solid H<sub>2</sub>**

Faraday Trans. 108 (in press) Special issue on "Dynamics of electronically Excited States"

F. Vigliotti, M. Chergui

Inst. de Physique Experimentale, Université de Lausanne, CH-1015 Lausanne, Switzerland

M. Dickgiesser and N. Schwentner

Inst. fuer Experimentalphysik, Freie Universitaet Berlin, D-14195 Berlin, Germany

Fluorescence and fluorescence-excitation spectra of the lowest Rydberg state of NO in H<sub>2</sub> matrices are presented. The intra- and intermolecular relaxation processes involving Rydberg states are discussed and modelled.

### **Assignment of the lowest excited states of C<sub>70</sub> and evidence for fluorescence from the S2 state**

J. Phys. Chem.A102 (1998) 3072

A. Sassara, G. Zerza and M. Chergui

Inst. de Physique Experimentale, Universite de Lausanne, CH-1015 Lausanne, Switzerland

Highly structured fluorescence, phosphorescence and fluorescence-excitation spectra of C<sub>70</sub> in neon matrices are reported. Fluorescence from both S1 and S2 states is observed and identified as states of A<sub>2</sub>' and E<sub>1</sub>' symmetry. A third singlet state is identified in the excitation spectrum and is proposed to be of A<sub>2</sub>' symmetry. Phosphorescence is due to a lowest triplet state of A<sub>2</sub>' symmetry.

### **Dynamics of Structural Relaxation upon Rydberg State Excitation of an Impurity in an Argon Crystal** Chemical Physics (in press), Special Issue on "Coherence in Chemical Dynamics"

S. Jimenez

Inst. de Physique Experimentale, Universite de Lausanne, CH-1015 Lausanne, Switzerland and IRRMA, CH-1015 Ecublens, Switzerland

A. Pasquarello, R. Car

Departement de Physique de la Matiere Condensee, Univ. de Geneve, Geneva, Switzerland and IRRMA, CH-1015 Ecublens, Switzerland

and M. Chergui

Inst. de Physique Experimentale, Universite de Lausanne, CH-1015 Lausanne, Switzerland

We present the results of a study aimed at describing the ultrafast dynamics of structural relaxation around a Rydberg excited NO molecule in an Ar crystal. Classical molecular dynamics simulations and normal mode analysis are used to describe the details of the dynamics. The results show a behaviour characterized by an impulsive expansion of the cage radius at short times (<250 fs), followed by oscillations of the cage radius over several picoseconds. The dynamics show a high degree of nuclear vibrational coherence.

### **Lifetime Lengthening of Molecular Rydberg states in the condensed phase**

J. Chem. Phys. (in press)

F. Vigliotti, G. Zerza, M. Chergui

Inst. de Physique Experimentale, Universite de Lausanne, CH-1015 Lausanne, Switzerland

J. Rubayo-Soneira

Instituto Superior de Ciencias y Tecnologia Nucleares, Quinta de Los Molinos, Apartado postal 6163, Ciudad de la Habana, Cuba

We report on lifetime lengthenings of a molecule in condensed media in the case of the NO A<sub>2</sub>S+(v=0) Rydberg fluorescence in inert gas matrices. In rare gas matrices, the fluorescence stems from two types of sites hereafter called red and main. The red site exhibits a lifetime lengthening with respect to the gas phase by up to 100 fluorescence stems from monosubstitutional sites. It exhibits lifetime increases from the gas phase value, to up to two orders of magnitude in the sequence H<sub>2</sub>-Ne(D<sub>2</sub>)-Ar-Kr-Xe. Furthermore, this change in transition moment is not observed in the absorption spectrum. Different mechanisms are presented to discuss the observations.

### **The role of surface corrugation in the rotational rainbow scattering of NO from Ag(111)**

J. Chem. Phys. (accepted)

Thierry Duhoo and Didier Lemoine\*

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

With a single direction of corrugation along the rigid surface and a rotationally cold (J=1/2,3/2) incident beam, a

Boltzmann plot of the final J distribution no longer exhibits a sharp oscillatory behaviour, in qualitative agreement with experiments. Notably, the low-J rainbow vanishes.

### **Quantum study of oriented NO scattering from Ag(111): orientational steering and effects of surface corrugation**

Chem. Phys. (submitted)

Didier Lemoine and Thierry Duhoo

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

Good agreement is obtained with the steric measurements of Kleyn, Stolte and coworkers. A time-resolved analysis of the NO-axis distribution reveals significant reorientation as the molecule reaches the repulsive wall of the interaction. This is at variance with a number of prior interpretations based on an impulsive collision model.

### **Crossed-beam reaction of carbon atoms with sulfur containing molecules I: Chemical dynamics of thioformyl (HCS; X<sup>2</sup>A) formation from reaction of C(<sup>3</sup>P<sub>j</sub>) with hydrogen sulfide, H<sub>2</sub>S(X1A1)**

J. Chem. Phys. (submitted)

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

### **Neutral-Neutral reactions in the interstellar medium II: isotope effects in the formation of l/c-C3H and C3D radicals in interstellar environments**

Astrophysical Journal (submitted)

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

### **Structural Changes in GaAs Induced by Ultrafast (fs) Laser Pulses**

Journal of Materials Research

L. Nnai, R. Vajtai, Cs. Beleznai, J. Remes, S. Leppvuori, and Thomas F. George\*

Office of the Chancellor / Departments of Chemistry and Physics and Astronomy, University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897

tgeorge@uwsp.edu Atomic force microscopy and Raman microprobe analysis of the laser-treated area show centrosymmetric (disordered) features which are different from the original zinc-blend structure of the GaAs lattice where the frozen-in structure shows evidence for a special heat transfer from the laser-induced crater to the boundary, namely the heat has been transferred ballistically by a high-density electron-hole plasma.

### **Exact Wave Function of a Harmonic Plus an Inverse Harmonic Potential with Time-dependent Mass and Frequency**

Physical Review A (Brief Reports)

Chung-In Um, Shang-Moon Shin, Kyu-Hwang Yeon, and Thomas F. George\*

Office of the Chancellor / Departments of Chemistry and Physics and Astronomy, University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897

tgeorge@uwsp.edu

Using canonical and unitary transformations and the Lewis-Risenfeld invariant method, the exact Schrodinger wave function for a harmonic plus inverse harmonic potential with time-dependent mass and frequency is obtained analytically.

### **Theoretical Studies of Atom-Surface Spectroscopy**

Recent Developments in Physical Chemistry (Transworld Research Network, Trivandrum, India)

Henk F. Arnoldus and Thomas F. George\*

Office of the Chancellor / Departments of Chemistry and Physics and Astronomy, University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897

tgeorge@uwsp.edu

Electronic properties of atoms are not only determined by the internal structure Hamiltonian, but also by the

environment of the atom. For the case of a metallic medium we compare the results for silver with the values for the perfect mirror where it appears that for a dipole oriented parallel to the surface of the substrate the correspondence is reasonable, but for a perpendicular dipole it is not.

### **Theoretical Treatment of Surface Adsorbates**

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

Lszl Nnai, Csaba Beleznai, and Thomas F. George\*

Office of the Chancellor / Departments of Chemistry and Physics and Astronomy, University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897

tgeorge@uwsp.edu

Theoretical and computational methods used to describe chemisorption and adsorbate reactions on solids, mainly metallic surfaces, are summarized, where the main focus is on electronic structural treatments of a one-electron nature, based on computational techniques in quantum chemistry.

### **Scattering of Aligned Molecules. The Potential Energy Surfaces for the Kr-O<sub>2</sub> and Xe-O<sub>2</sub> Systems**

J.Chem.Phys., in press (1998)

Vincenzo Aquilanti, Daniela Ascenzi, David Cappelletti, Miguel de Castro, and Fernando Pirani  
Dipartimento di Chimica - Università di Perugia, I-06123 Perugia, Italy

### **A Theoretical Study of Core Excitation Spectra of NO Molecule**

J. Phys.B: Atomic, Molecular & Optical Physics (in print)

F. Wang and F. P. Larkin

School of Chemistry, The University of Melbourne, Parkville, Victoria 3052, Australia.

### **Theoretical Study of Excitation and Radiative De-excitation: Characteristics for the NO Molecule**

J. Phys.B: Atomic, Molecular & Optical Physics (submitted)

F. Wang and F. P. Larkins

School of Chemistry, The University of Melbourne, Parkville, Victoria 3052, Australia.

### **Influence of Ground State Geometry on Carbon Monoxide: X-ray Emission Spectral Profile**

J. Phys.B: Atomic, Molecular & Optical Physics (submitted)

F. Wang and F. P. Larkins

School of Chemistry, The University of Melbourne, Parkville, Victoria 3052, Australia.

### **Microwave spectra of the Ne-N<sub>2</sub> Van der Waals complex: experiment and theory**

J. Chem. Phys. (submitted)

W. Jäger<sup>a</sup>, Y.Xu<sup>a</sup>, G. Armstrong<sup>a</sup>, M.C.L. Gerry<sup>b</sup>, F. Y. Naumkin<sup>c</sup>, F. Wang<sup>c†</sup> and F.R.W. McCourt<sup>c</sup>

<sup>a</sup>Department of Chemistry, University of Alberta, Edmonton, Alberta, T6G 2G2, Canada

<sup>b</sup>Department of Chemistry, University of B.C., Vancouver, B.C., V6T 1Z1, Canada

<sup>c</sup>Department of Chemistry, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada

† current address: School of Chemistry, The University of Melbourne, Parkville, Victoria 3052, Australia.

### **Metastable hydrogen atom scattering by crossed molecular beams: total cross sections for H\*(2s)-Kr, O<sub>2</sub> and Cl<sub>2</sub> at thermal energies**

Chem. Phys. Lett. (in press)

Brunetto G. Brunetti<sup>‡</sup>, Pietro Candori<sup>‡</sup>, Jaime De Andres<sup>\*</sup>, Stefano Falcinelli<sup>#</sup>, Marta Stramaccia<sup>‡</sup> and Franco Vechiocattivi<sup>#</sup>.

<sup>‡</sup> Dipartimento di Chimica, Università di Perugia, 06123 perugia, Italy

<sup>\*</sup> Departament de Química Física, Universitat de Barcelona, 08028 Barcelona, Spain

<sup>#</sup> Istituto per le Tecnologie Chimiche, Università di Perugia, 06123 Perugia, Italy

The velocity dependence of total integral cross sections for collisions of  $H^*$  (2s) atoms with Kr,  $O_2$ , and  $Cl_2$  has been measured, in the velocity range from 4 to 40  $Km\ s^{-1}$ , in a crossed molecular beam apparatus. The results have been obtained in an experimental configuration with a detector acceptance angle well below the minimum critical angle, allowing a comparison with quantum mechanical cross section calculations.

### **Penning ionization of $C_{60}$ molecules**

Chem. Phys. Lett. (submitted)

B. Brunetti, P. Candori, R. Ferramosche

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

S. Falcinelli, F. Vecchiocattivi

Istituto per le Tecnologie Chimiche, Università di Perugia, 06123 Perugia, Italy

A. Sassari, M. Chergui

Institut de Physique Expérimentale, Université de Lausanne, CH-1015 Lausanne-Dorigny, Switzerland

A mass-spectrometric study of Penning ionization of  $C_{60}$  with metastable rare gas atoms ( $Rg = He, Ne, Ar, Kr$  and  $Xe$ ) shows that in all cases the sole channel is  $C_{60}^+$  formation. The ionization cross sections, at an average collision energy of 0.05 eV, strongly decrease going from helium to xenon. The interaction potentials for  $C_{60}-Rg^*$ ,  $C_{60}^+-Rg$ ,  $C_{60}-Rg$ ,  $C_{60}^- -Rg^+$ , as well as matrix elements for the coupling of  $C_{60}-Rg^*$  and  $C_{60}^- -Rg^+$  interactions at the crossing point, have been estimated by using recently proposed correlation formulas. The observed trend of the ionization cross sections can be explained taking into account that the low energy collisions between  $Rg^*$  and  $C_{60}$  are characterized by the formation of an ion-pair  $C_{60}^- -Rg^+$  intermediate with a decreasing probability going from lighter to heavier rare gases.

## **c. Conferences**

### **1. 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.

### **2. 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).

### **3. 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>

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

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

Thanks to the large participation expected for the 21st RGD, covering a wide range of topics, we hope to gather together again the MB people and the RGD people, as in the past decades. A complete information on the RGD-21 including program, papers, registration and accomodation is given in our second announcement and kept up to date on our Web site at:

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

The Molecular Beam session will be held in the style of the MB symposia, with oral papers including about 25 invited lectures, and poster papers. The list of the invited speakers to the MB session will be available soon.

This special announcement is made with the agreement and the strong support of the Secretary (U. Buck) and the Members of the International Advisory Committee of the Molecular Beam Symposia. Organizers of the MB session are: V.Aquilanti (Perugia), E.L. Knuth (UCLA), P. Toennies (Gottingen) and R. Campargue (co-Chairman, RGD-21).

Please note that, because the announcement of the MB session has been sent lately, the deadline for submission of abstracts is extended accordingly up to May 25, 1998. Nevertheless, for simplifying the scientific organization of the Symposium, all the potential contributors are invited to transfer as soon as possible by e-mail their name(s), affiliation(s) and abstract title(s). They will receive immediately one or a range of abstract numbers. The complete information for the preparation of the two-page abstract is available on our Web site.

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

### **5. 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.

## **6. 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.

## **7. NEW TRENDS IN CHAOS THEORY**

Summer School August 3-7 1998, El Escorial, Madrid (Spain)

Organized under the auspices of: Fundacion General de la Universidad Complutense, Digital, and Hewlett-Packard.

Chairman: F. Borondo Dep. de Quimica, C-IX; Universidad Autonoma de Madrid; CANTOBLANCO – 28049 Madrid, Spain

Secretary: R.M. Benito, Dep. de Fisica y Mecanica; ETSI Agronomos; Univ. Politecnica de Madrid; Madrid (Spain)

Lecturers: O. Bohigas (CNRS, Orsay), A. Fernandez (Tribunal de Cuentas, Madrid), T. Geisel (MPI, Goettingen), M.C. Gutzwiller (IBM and Univ. of Yale), J. Laskar (Bureau des Longitudes, Paris), A. Martin-Pereda (Univ. Politecnica, Madrid), S. Miret-Artes (CSIC, Madrid), F. Moran (Univ. Complutense, Madrid), M. Rubi (Univ. Barcelona), M. San Miguel (IMEDEA, Univ. Islas Baleares), J. Santamaria (Univ. Complutense), T. Uzer (Georgia Tech, Atlanta).

Scientific Programme: The course will cover manifestations of chaos in different fields: Random Matrix Theory, Economy, Mesoscopic Systems, Quantum Chaos, Chaos in the solar system, Biological systems, Stochastic resonances, Spatio-Temporal Chaos, Atoms in external fields, Scars.

Registration: The school is opened to 60 graduate students and post-doctoral young researchers, both theoretical and experimental, in the field of non linear science. The registration fee is 19,000 Spanish Pesetas. Lodging and full board is available at the price of 46,000 Spanish Pesetas. About 15 grants, from the Complutense University, are available for students and post-docs under request. Deadline for registration: July 1, 1998. Deadline for grant applications : June 5, 1998; candidates should contact: [f.borondo@uam.es](mailto:f.borondo@uam.es), [rbenito@fis.etsia.upm.es](mailto:rbenito@fis.etsia.upm.es)

tel: +34 91 3974964, +34 91 3365646, fax: +34 91 3974187

Information also available in the web: <http://fis26.fis.etsia.upm.es/Escorial>

## **8. PHOTODYNAMICS OF MOLECULES AND CLUSTERS**

Summer School August 10-15 1998, El Escorial, Madrid (Spain)

Organized under the auspices of: Chemical Physics Section of the Atomic and Molecular Physics Division (EPS), Universidad Complutense de Madrid, Consejo Superior de Investigaciones Cientificas

Chairman: Gerardo Delgado-Barrio, Secretary: Pablo Villarreal, Instituto de Matematicas y Fisica Fundamental, C.S.I.C., C/ Serrano 123, 28006-Madrid, Spain

Lecturers: E. Aquilanti (Perugia), J.A. Beswick (Toulouse), M. Chergui (Lausanne), G. Delgado-Barrio

(C.S.I.C.), A. Gonzalez Ureña (Madrid), K.C. Janda (Irvine), J. Jellinek (Argonne), O. Roncero (C.S.I.C), P. Villarreal (C.S.I.C.)

Scientific Programme: Spectroscopy and dynamics of elementary reactions in clusters and crossed-beam experiments. Molecular beam techniques for the study of intermolecular interactions. Liquid helium nanodroplets: a new medium for chemical physics studies. Density matrix propagation and stationary absorption spectra, and photodissociation of molecules in rare gas matrices. Quantum, classical and hybrid methods to study the Predissociation of van der Waals clusters. Small boson systems. Reactive collisions and photoinitiated reactions.

Registration: The school is opened to 60 graduate students and post-doctoral young researchers, both theoretical and experimental, in the field of atomic and molecular physics. The registration fee is 19,000 Spanish Pesetas. Lodging and full board will be 43,000 Spanish Pesetas. About 15 grants, from the Complutense University, are available for students and post-docs under request. Before June 15th, candidates are invited to contact with:

gerardo@cc.csic.es, pablo@cc.csic.es

tel: +34 91 5901607, +34 91 5901610, fax: +34 91 5854894

Information also available in the web: <http://www.imaff.csic.es/fam/famnove.html>

## **9. 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.

## **10. MOLECULAR PHYSICS OF STRUCTURE AND CHANGE**

Lunteren, The Netherlands, September 2-4, 1998

The 3rd European Meeting of the Molecular Beams and Dynamics Group will be held in Lunteren, The Netherlands from September 2 till September 4 1998 and will be organized by the Section Atomic Physics and Quantum Electronics of the Dutch Physical Society.

Sponsors are the Dutch Physical Society (NNV) and the Foundation for Fundamental Research on Matter (FOM). The British Council in The Netherlands and the Faraday Division of the Royal Society of Chemistry has allocated funds to support the travel of young scientists from the U.K. to the meeting.

### **ADVISORY COMMITTEE**

W.J. van der Zande (AMOLF, organizer), B.J. Whitaker (Leeds, organizer), M.N.R. Ashfold (Bristol), A.J. Orr-Ewing (Bristol), K.L. Reid (Nottingham), K. Bergmann (Kaiserslautern), D.H. (Nijmegen), M. Vrakking (AMOLF)

### **AIM OF THE MEETING**

A particular aim of the meeting is to provide a forum for graduate students and postdoctoral researchers (as well as more senior scientists) to meet, learn, exchange knowledge, present results and establish new contacts, in an informal setting. The format of the meeting will be similar to that of the previous European meetings of the Molecular Beams and Dynamics Group in Orsay (1992) and Kaiserslautern (1995), with a strong emphasis on contributions from graduate students and interactions between the participants.

The scientific programme, which will run from 18.00 hours on Wednesday September 2 till 18.00 hours on Friday September 4, includes all aspects of molecular structure and molecular dynamics in the gas phase, at interfaces and in liquids. Sessions will be opened by an overview lecture from a distinguished scientist, who will concentrate on unresolved issues in the field. Short presentations will be selected from contributions from younger scientists, among which a few hot topics will be chosen for a longer contribution. Poster sessions will be scheduled for additional presentations. We hope that all participants will be willing to present their work. Discussion will be encouraged explicitly by allocating ample discussion time during the oral sessions.

INVITED SPEAKERS Dr. A.J. Orr-Ewing (Bristol): Predissociation dynamics using cavity ring-down spectroscopy

Professor D.H. Parker (Nijmegen): Velocity Imaging studies of diatomic molecule photodissociation

Professor J. Vigue (Toulouse): Index of refraction of gases for atomic waves: measurements and calculations

Professor L. Wöste (Berlin): Real Time observation of structural changes in small molecules by means of femtosecond spectroscopy

#### HOW TO APPLY:

The meeting format and anticipated spirit of the conference, as well as the available facilities, limits the number of participants to 100. Early application is thus recommended.

The application should include: A tentative title of the anticipated contribution dealing with a research topic within the general scope of the meeting. Please indicate a preference for oral/poster. (A one page -camera ready- abstract is due by June 1, 1998). \* Your postal address, \* Your e-mail address, \* A fax number (if available), If you are applying for a travel bursary you must also include a brief supporting statement from your supervisor.

Send your application to MBDG Secretary: Ms. Magda Speijers, Molecular and Laser Physics University of Nijmegen PO Box: 9010 NL 6500 GL Nijmegen The Netherlands (Magdas@sci.kun.nl)

#### TRAVEL:

Lunteren is situated near the geographic centre of The Netherlands. The conference center is within walking distance (15 min.) of the local train station of Lunteren and is situated in a quiet, wooded area. The travel time by train from major train stations in The Netherlands such as Schiphol, Amsterdam, Rotterdam and Nijmegen is roughly 1.5 hours. De Blije Werelt can be found on internet <http://www.blijewerelt.nl/> with detailed information on location and travel.

#### ACCOMMODATION AND REGISTRATION:

A fee of Dfl. 350,- will apply to all participants to cover the cost of the book of abstracts, and full room and board for two days. Fee must be paid upon arrival at the conference. The conference starts with a dinner on Wednesday September 2 and ends before dinner on September 4.

#### TRAVEL SUPPORT:

It is expected that most participants will cover their expenses from funds provided by their institutions. However, young scientists from the U.K. may apply for partial support from funds made available by the British Council in the Netherlands and the Faraday Council. Interested and eligible candidates should contact Dr. B.J. Whitaker, Secretary of the MBDG, University of Leeds, Leeds LS2 9JT, U.K. by post, fax (44 113 233 6565) or, preferably, by e-mail (benw@chem.leeds.ac.uk).

#### THE SECOND ANNOUNCEMENT:

The second announcement which will contain the final program, will be sent out early August to all those who have applied. Applicants will be contacted by the advisory committee concerning their placement in the oral or poster program by e-mail as soon as possible.

#### CONFERENCE SECRETARIAT:

All correspondence (except as specified otherwise above) should be sent to:

MBDG Conference Secretariat, Ms. Magda Speijers, Prof. W.J. van der Zande, Molecular and Laser Physics, University Nijmegen, PO Box: 9010, NL 6500 GL Nijmegen, The Netherlands

Magdas@sci.kun.nl

#### DATES AND DEADLINES:

Apply as soon as possible, but no later than June 1, 1998 Abstracts due by June 1, 1998 A second announcement and final programme will be sent out early July

**11. 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)).

### **12. 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 ([qfpcaalf@lgdx02.lg.ehu.es](mailto:qfpcaalf@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)

### **13. 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)

### **14. 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>

### **15. STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS**

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

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

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

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

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

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

- \* Demonstrations of active or coherent control of chemical processes

At this time we are seeking Titles and Abstracts of about 300 words. The DEADLINE for submission of these proposed contributions is FRIDAY 29 MAY 1998. They should be sent to Dr. BJ Whitaker, School of Chemistry, University of Leeds, LS2 9JT and may be in any form - manuscript, fax, whatever but electronic attachments will be particularly cherished. Papers should be concerned with new, unpublished work. The full proceedings of the Discussion will be published late in 1999, but papers accepted for discussion will be circulated to all participants before the meeting in July 1999. Those unfamiliar with the unique format of Faraday Discussions can obtain more information from the URL above.

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

**16. 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

## **Special announcement**

To the memory of

**Professor Roger Grice**

(1941 - 1998)

A meeting will be held on the afternoon of Monday 14th September 1998 in the Chemistry Department, Manchester University. This meeting will include recollections and scientific contributions related to Roger's work and provide the opportunity for Roger's former students, colleagues, collaborators and friends to commemorate his scientific achievements and remember his life.

The meeting will be preceded by a buffet lunch and will be attended by members of the family. It is also planned to launch an appeal to establish a prize or scholarship in Roger's memory at this time.

If you wish further details of the meeting, please contact

Dr J C Whitehead

Chemistry Department

Manchester University

Manchester M13 9PL.

(Tel: 0161-275 4692; Fax: 0161- 275 4598; e-mail: [j.c.whitehead@man.ac.uk](mailto:j.c.whitehead@man.ac.uk))

Sponsored by the Molecular Beams and Dynamics Group of the Royal Society of Chemistry.