

Molecular Dynamics News

number 94, April 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 has been accepted - otherwise state *unpublished*).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 95 to Prof. V. Aquilanti (You are encouraged to use electronic mail: AQUILA@HERMES.CHM) (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#94). The closing date for issue number 95 is June 1, 1998.

* 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**

Name: _____
Address: _____

Electronic Mail Address (optional): _____

WWW Address (optional): _____

Fax Number (optional): _____

Delivery Method: Hardcopy _____ Email(PostScript) _____ Email(LaTeX) _____ Mosaic _____

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

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 a 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

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.

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. Reserach 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

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 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 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, <http://www.lbl.gov/agsuits>

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 addresses 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 (Cl_2 , CH_3Br , CH_3I)
2. Multiphoton Dissociation of molecules (CS_2 , NO_2 , CH_3I)
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 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 CS_2 USING ION IMAGING, P.C. Samartzis and T.N. Kitsopoulos, J. Phys.Chem. 101, 5620 (1997).

3. PHOTOFRAGMENTATION OF Cl_2 AT 308 NM, P.C. Samartzis, T. Gougousi, and T.N. Kitsopoulos, Laser Chem. 100, 1 (1998).

4. PHOTODISSOCIATION STUDY OF CH_3Br 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
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 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 phone: (412)396-4732 or by FAX: 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 an 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(¹D) 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(²D), N(⁴S), and O(³P) 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 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 or 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.* 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) 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. 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 ($M^+ \cdot R_x$, where $M = \text{Mg, Ca, Ti, etc.}$ and $R = \text{Ar, CO}_2, \text{H}_2\text{O, N}_2, \text{C}_2\text{H}_2, \text{etc.}$) 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 $\text{Ca}^+ - \text{N}_2$," *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

Hyperspherical elliptic coordinates for the theory of light atom transfer reactions in atom-diatom collisions

J. Chem. Phys.

O. I. Tolstikhin and H. Nakamura*

Division of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444, Japan

The new coordinate system, hyperspherical elliptic coordinates, is introduced to study quantum dynamics of

light-heavy-light reaction systems. Its power and efficiency are demonstrated by $O(3P)+HCl$ reaction as an example.

Quantum mechanical elucidation of reaction mechanisms of heavy-light-heavy systems: Role of potential ridge

J. Chem. Phys.

K. Nobusada, O.I. Tolstikhin, and H. Nakamura*

Division of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444, Japan

Vibrationally adiabatic potential ridge is successfully introduced for 3D reactions, and quantum reaction mechanisms are clarified with the help of potential ridge and nonadiabatic transitions at avoided crossings.

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, Université 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, Université 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.

Cu^{++} and Li^{+} interaction with polyethylene oxide by ab initio Molecular Dynamics.

J. Chem. Phys.

Amedeo Palma*, Alfredo Pasquarello+, Giovanni Ciccotti and R. Car+.

ICMAT-CNR, Via Salaria Km 29.5, I-00016 Monterotondo S. (RM) Italy.

+ IRRMA, Ecublens, CH-1015 Lausanne, Switzerland and Dept. of Condensed Matter Physics, University of Geneva, CH-1211.

INFN - Dip di Fisica Università di Roma I, P. A. Moro 2, Roma.

Equilibrium positions on the Li^{+} PEO and Cu^{++} PEO ground state potential energy surfaces have been determined by ab initio MD. The energy barriers for Li^{+} and Cu^{++} ionic diffusion along the PEO chain have been estimated.

Hyperspherical symmetry of hydrogenic orbitals and recoupling coefficients among alternative bases

Phys. Rev. Lett. 80(1998) 3209

Vincenzo Aquilanti, Simonetta Cavalli, Cecilia Coletti

Dipartimento di Chimica dell'Università, 06123 Perugia, Italy

Fock's representation of momentum space hydrogenic orbitals in terms of harmonics on the hypersphere S^3 of a four dimensional space is extended to classify alternative bases. These orbitals are of interest for Sturmian expansions of use in atomic and molecular structure calculations and for the description of atoms in fields. Due to the correspondence between the S^3 manifold and the $SU(2)$ group new sum rules are established which are of relevance for the connection, not only among hydrogen atom orbitals in different bases, but also among usual vector coupling coefficients and rotation matrix elements.

Quasiclassical trajectory method for molecular scattering processes: necessity of a weighted binning approach

Chem. Phys. Lett. 277(1997) 183

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moléculaire, URA 5803, Université Bordeaux I and CNRS, 33405 Talence Cedex, France

It is shown that the standard binning method utilized in the classical study of scattering processes dealing with more than three atoms, is not appropriate when the total energy disposal in the products is too low for the classical and quantum densities of vibrational states to be equal. Two simple semiclassical corrections are proposed.

Some new aspects of product distribution functions for three-atom unimolecular reactions performed in beam experiments

J. Phys. Chem. A 1997, 101, 9318

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moleculaire, URA 5803, Universite Bordeaux I and CNRS, 33405 Talence Cedex, France

Energy distribution functions for the products in two classes of three-atom unimolecular reactions are derived which are much more realistic than the prior distributions of Levine and Bernstein without being more complicated. In a first step, we deal with light-atom emissions governed by short-range forces and in a second step, with processes governed by long-range forces. Comparison is done with experimental results or results of simulations.

A model of rotational-translational energy transfer in the exit-channel of a three-atom unimolecular reaction

C. R. Acad. Sci. Paris, t. 1, Serie II c, p. 101, 1998

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moleculaire, URA 5803, Universite Bordeaux I and CNRS, 33405 Talence Cedex, France

For a three-atom unimolecular reaction of the type $ABC \rightarrow AB + C$ performed in a supersonic beam experiment, we propose an analytical model to describe how the rotational angular momentum of AB varies from the transition state onto the separated products.

On the possibility of excited recoil energy distributions in the products of complex-forming reactions with no exit-barrier

J. Phys. Chem. A

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moleculaire, URA 5803, Universite Bordeaux I and CNRS, 33405 Talence Cedex, France

For some complex-forming processes governed by long-range forces, the kinematics are such that the recoil energy distribution may be very excited, despite the absence of exit-barrier, i.e., of repulsion forces between nascent fragments.

On the analysis of exit-channel effects in three-atom unimolecular reactions

Eur. Phys. J. D (to be published)

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moleculaire, URA 5803, Universite Bordeaux I and CNRS, 33405 Talence Cedex, France

The key problem of exit-channel effects in unimolecular reactions, which make Transition State Theory generally unsuitable for the calculation of product state distributions, is analysed in some details in the triatomic case, for a total angular momentum equal to zero.

Statistical analysis of the recoil energy distributions in the products of the unimolecular dissociations of NO_2 and C_2O

Chem. Phys. Lett. (submitted)

L. Bonnet and J.C. Rayez

Laboratoire de Physicochimie Moleculaire, URA 5803, Universite Bordeaux I and CNRS, 33405 Talence Cedex, France

The recoil energy distributions in the products of the title reactions are derived within the framework of Phase Space

Theory (PST). The strong fluctuations observed experimentally, in contrast with the smooth character of the bell-shaped distributions usually observed in bimolecular complex-forming processes, are analysed.

Production and magnetic analysis of beams of S atoms and SO radicals. A collisional study of their interactions with hydrogen molecules

Int. J. Mass Spectrom. & Ion Processes, in press (1998)

Vincenzo Aquilanti, Daniela Ascenzi, Elisabetta Braca and David Cappelletti

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

Stern-Gerlach magnetic analysis indicates that both species are generated mainly in their electronic ground state and in the case of sulfur atoms with fine-structure levels populated according to their degeneracies. The analysis of experimental data (cross sections and their velocity dependence, which exhibits glory interference patterns) allows a characterization of the spherically average component of the interaction potentials. A discussion of the effect of the Σ - Π splitting, spin-orbit and electrostatic (including quadrupole-quadrupole) interaction on the dependence of the hydrogen molecule orientation is given for the S-H₂ potential energy surface.

Hyperquantization algorithm. I. Theory for triatomic systems

J. Chem. Phys. (1998)

V. Aquilanti, S. Cavalli and D. De Fazio

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

Angular momentum algebra is generalized to compute matrix elements of the Hamiltonian operator parametrically in the hyperradius. Advantages are that no integrals are required and the construction of the kinetic energy matrix is simple and universal: salient features are the block tridiagonal structure, a number of symmetry properties and sparseness.

Hyperquantization algorithm: II. Implementation for the F + H₂ reaction dynamics including open-shell and spin-orbit interaction

J. Chem. Phys. (1998)

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

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

A. Aguilar, X. Gimenez, J. M. Lucas

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

Numerical aspects and performances of the hyperquantization algorithm (preceding paper) for this prototypical atom-diatom reaction at total nuclear angular momentum equal to zero. The extensions which allow the treatment of excited electronic surfaces are provided, the fine structure of the fluorine atom being explicitly taken into account.

c. Conferences

1. 53rd OHIO STATE UNIVERSITY INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY

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

The preliminary program for the 53rd Ohio State University Symposium on Molecular Spectroscopy to be held June 15-19, 1998, in Columbus, Ohio, is now available for viewing (click on "Meeting Program" on the home page) at the Symposium WWW site with the following address:

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

It contains the times of all scheduled talks as well as other valuable information. Copies in several formats may also be downloaded for local printing from the web site or via anonymous FTP

(molspect.mps.ohio-state.edu and in the symposium directory). Please consult the README file on the WWW or FTP site for details about available formats.

Please contact the Symposium directly for program information if you need further assistance: Phone:

(614)292-2569; FAX: (614)292-1948; email: mss@molspect.mps.ohio-state.edu

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

2. 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. Bultjies (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 quantum 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 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>

3. 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

4. International Conference on WATER IN THE GAS PHASE

University of Marne la Vallee, PARIS, FRANCE, June 21-24, 1998

The conference on "Water in the Gas Phase" will deal with a wide range of scientific aspects of the properties and structure of water and water nanoclusters in the gas phase. Topics which are in the areas of astrophysical and spectroscopic studies will form a major part of the conference presentations; stress will also be placed on studies of reactivity and dynamics. In all of these areas, emphasis will be given to both experimental and theoretical efforts.

Confirmed Speakers: WATER

Jacques Crovisier, Observatoire of Paris, France "H₂O in comets"

Michel Desbois, Ecole Polytechnique, Palaiseau, France "Water vapor in the atmosphere: radiative effects and role on the climate system"

Peter Bernath, University of Waterloo, Canada "Laboratory spectroscopy of water"

Oleg Polyansky, UCL, U.K. "Analysis of hot water spectra in sunspots and the laboratory"

Claude Camy-Peyret and Jean-Marie Flaud, University of Orsay, France "Low pressure flame H₂O spectra"

Jonathan Tennyson, UCL, U.K. "First principle calculation of the spectrum of hot water"

David Schwenke, NASA, Ames Field, U.S.A. "Ab initio calculations of water line strengths"

Larry Rothman, Harvard-Smithsonian Center, U.S.A. "Evaluation of water vapor line-parameter databases: HITRAN and HITEMP"

Laurent Coudert, University of Orsay, France "Spectroscopy of water vapor: the rotational energy pattern of a floppy triatomic molecule"

Wilfried Meyer, University of Kaiserslautern, Germany "Dynamic polarisabilities of water and long range interactions" Fleming Crim, University of Wisconsin, U.S.A. "Using vibrations of water to control bimolecular reactions and photodissociation"

Reinhard Schinke, MPI Goettingen, Germany "Photodissociation of water"

Barry L. Lutz, Northern Arizona University, U.S.A. "H₂O⁺ in comets"

Michel Vervloet, Universite of Orsay, France "Spectroscopy of H₂O⁺"

Pavel Rosmus, UMLV, France "Renner-Teller spectra and transition probabilities of H₂O⁺"

WATER NANOCLUSTERS Friedrich Huisken, MPI Goettingen, Germany "Vibrational spectroscopy of free and adsorbed water clusters"

David Nesbitt, JILA, Boulder, USA "Breaking bonds in water and water clusters: zero point and vibrationally mediated photofragmentation dynamics"

Welford Castleman, Pennsylvania State University, U.S.A. "Solvation effects on reactions in clusters"

Samuel Leutwyler, University of Bern, Switzerland "Structures, isomers and torsional interconversions of small water clusters"

Richard Saykally, UC, Berkeley, U.S.A. "Studies of water clusters by terahertz and IR cavity ringdown spectroscopy: force fields"

Bernd Brutschy, University of Frankfurt, Germany "Water clusters attached to benzene derivatives: structure, binding, energies, ion-chemistry"

Udo Buck, MPI Goettingen, Germany "Excitation spectra of intra- and intermolecular motions of water clusters"

Leo Lehr, University of Munich, Germany "Dynamics in I₂(H₂O)_n clusters"

Michele Parrinello, MPI Stuttgart, Germany "Ab initio simulation of proton transfer and water clusters"

Ad van der Avoird, University of Nijmegen, The Netherlands "Tunneling dynamics and spectra of water clusters"

Claude Leforestier, Universite of Montpellier, France "VTR energy transfer of water dimer: influence of the internal vibrations"

Zlatko Bacic, New York University, U.S.A. "Quantum dynamics of coupled torsional vibrations in (H₂O)₃, (H₂O)₄ and their isotopomers: energy levels, tunneling splittings and vibrationally averaged rotational constants"

Gereon Niedener-Schatteburg, University of Munich, Germany "Reactivity of charged water clusters"

Martin Schuetz, University of Stuttgart, Germany "Local treatment of electron correlation in water clusters"

Franco Gianturco, University of Roma, Italy "Structure and dynamical aspects of proton water interaction and energy transfer"

Jim Coe, Ohio State University, U.S.A. "OH⁻ and H₃O⁺ recombination as a function of water solvent"

Kit Bowen, John Hopkins University, U.S.A. "Water dipole cluster anions studied by photoelectron spectroscopy"

Mark Johnson, Yale University, U.S.A "Electron and ion hydration in clusters"

Suehiro Iwata, IMS, Okazaki, Japon "Structure and spectroscopy of water cluster anions"

Sotiris Xantheas, Pacific Northwest National Laboratory, U.S.A. "Interplay between cooperativity and hydrogen bonding network in water clusters"

Elise Kochansky, University of Strasbourg, France "Study of electronic states of H₅O₂⁺"

Peter Rossy, University of Texas, U.S.A. "Solvent clustering in supercritical water"

Mike Klein, University of Pennsylvania, U.S.A "Ab initio studies of acid/water clusters"

LOCAL ORGANIZING COMMITTEE

Paul Bagus, Gilberte Chambaud, Pavel Rosmus, Universite de Marne-la-Vallee, 5 boulevard Descartes (Bat. M2), F-77454 Champs sur Marne, Cedex 2, France, Tel. +33-1-60957304 /FAX +33-1-60957320, e-mail: h2o@alpha.univ-mlv.fr

Deadline for final registration and submission of abstracts: May 1st 1998. Participants are invited to submit

abstracts for short oral and for poster presentations. 3rd circular with meeting information: End of May 1998.
WWW home page: <http://alpha.univ-mlv.fr:8080/waterconference.html> Precedence: list

5. 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

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, 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

6. The 1998 Gordon Research Conference on ATOMIC AND MOLECULAR INTERACTIONS

Conference Chair: Bob Wyatt (wyatt@quantum.cm.utexas.edu), Vice-Chair: David Chandler (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!!

7. 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 0AJ (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

8. 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 or fax 39-75-5855606.

9. 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).

10. 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>

11. 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

12. 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 Website: <http://www.conferences.ubc.ca/theochem.htm>

Deadline for Abstracts June 1, 1998.

13. 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.

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

14. 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>

15. 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 CO₂ 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_3^+ 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](ftp://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.

16. MOLECULAR PHYSICS OF STRUCTURE AND CHANGE

Lunten, The Netherlands, September 2-4, 1998

The 3rd European Meeting of the Molecular Beams and Dynamics Group will be held in Lunten, 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

17. 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).

18. 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) or from the Gas Kinetics Group Secretary, Dr J.M.C. Plane, E-mail: 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

19. 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

20. 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/chimngen/mb/cong/comet.html>

21. 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

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

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)

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