

# Molecular Dynamics News

*numbers 100,101,102; April, June, August 1999*

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

The format for MDN is

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 has been accepted - otherwise state *unpublished*).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

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

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

Send all material for issue 103 to Prof. V. Aquilanti (**You are encouraged to use electronic mail: AQUILA@DYN.UNIPG.IT**). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#102). The closing date for issue number 103 is October 1, 1999.

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

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

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

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## MESSAGE FROM THE EDITORS

Molecular Dynamics News has now published more than 100 issues since Dick Zare and Raphi Levine started the newsletter in 1982. We have witnessed great progress in the field during this time because of advances in experimental techniques as well as extraordinary improvements in the speed and capabilities of computers that has been exploited by new theoretical and computational approaches. Now the advances in computational capability have opened a whole branch of Molecular Dynamics dealing with simulations even in liquid and solids, which has grown up outside the scope of the newsletter. Even the avenues for the dissemination of timely scientific information has progressed enormously, and we have exploited that. Now most of our subscribers get the issue by email or read it on the web. For a few years we also have, on the initiative of Jeremy Hutson, a complementary email list. We take the occasion of celebrating the 100th issue to thank all those who have helped by subscribing and submitting contributions. We are confident that you will continue to contribute, so as we feel encouraged to continue publishing the newsletter into the next millenium.

We are also sorry for the production problems that have interrupted timely publication of this newsletter for the past two issues. We believe that these problems have now been resolved. This issue contains all information that would have been published in April and June except for Conferences that have already occurred and were previously announced in MDN and expired job postings.

## ELECTRONIC DELIVERY OF MDN

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

### 1. Electronic mail to subscribers

In this case subscribers tell us if they want the newsletter automatically sent to them by electronic mail. Subscribers may specify whether they want a raw LaTeX source file or a Postscript file.

### 2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file at the Molecular Dynamics News Web site: <http://www.ucsc.edu/mdn> A Web browser with suitable viewers allows people to read the files on their computer screens. Alternatively the files can be downloaded for local viewing or printing. Subscribers choosing this delivery option will receive an email announcement when a new issue is posted.

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

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

#### MOLECULAR DYNAMICS NEWS EMAIL LIST

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

Santa Clara, a Jesuit university located in Silicon Valley and ranked second by U.S. News among regional universities in the West, seeks a person to teach non-science majors courses (University Core), lower division service courses and advanced courses in physical chemistry. Ph.D. required. A vigorous undergraduate research program is expected. Demonstrated excellence in teaching and research essential. Our ACS-approved department is well-equipped, including an x-ray diffractometer and 400 MHz NMR. For additional information: <http://chem.scu.edu>. Send CV, transcripts, three letters of recommendation, statements of teaching philosophy and research plans, and cover letter to Dr. Brian McNelis, Chemistry Department, 500 El Camino Real, Santa Clara University, Santa Clara, CA 95053 by October 7, 1999. Santa Clara University is an equal opportunity/affirmative action employer, and welcomes applications from women, persons of color, and members of other historically underrepresented U.S. ethnic groups.

### **POST DOCTORAL AND VISITING**

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

(Re-advertisement due to withdrawal of a candidate)

A postdoctoral research assistantship is available to start as soon as possible to work on an National Environmental Research Council funded project entitled 'Computational analysis of water absorptions at near infrared and optical wavelengths'. The project will involve the first principles computation of water vibration-rotation spectra using programs developed at UCL, analysis of laboratory spectra, estimation of total atmospheric absorption by water and the construction of a reliable database of water transitions. The appointment will be at the lower end of the Research Staff Scale 1A, currently £15,735 - 23,651 per annum, depending on age, qualifications and experience plus £2,134 London weighting. The grant is for two years although it is College policy to appoint for one year in the first instance.

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

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

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

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

#### **POSTDOCTORAL POSITION, University of Osnabrueck**

A postdoctoral position (BAT IIa) is available in the field of cluster physics at the Department of Physics of the University of Osnabrueck for three years with special emphasis on Size Effects in Free and Deposited Clusters.

The experimental work concerns the construction and testing of cluster sources for producing variable size clusters. Size effects will be characterized using synchrotron radiation in the soft and hard X-ray regime. Detection techniques include mass spectrometry, photoelectron spectroscopy, and coincidence spectroscopies. Deposited clusters will be characterized using scanning tunnel microscopy, optical spectroscopy, and photoelectron spectroscopy. The experimental results will be interpreted using model calculations. Applicants should have experience in the above mentioned fields. They should also be

motivated to participate in interdisciplinary collaboration projects and beam line construction at the new storage ring BESSY-II (Berlin). Applicants are required to assist in teaching of students and they should have a diploma or equivalent degree in physics or chemistry as well as a Ph.D. in physics or physical chemistry. The University of Osnabrueck endeavors to employ a higher portion of female academic staff. Female candidates are therefore encouraged to apply, and will be selected if suitably qualified. Physically handicapped applicants will take precedence if equally qualified.

Applications containing the customary documents should be sent by 29.01.1999 to the Dekan des Fachbereichs Physik, Universitaet Osnabrueck, Barbarastr. 7, D-49069 Osnabrueck, Germany.

#### **POSTDOCTORAL POSITION, University of Toronto**

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

Please call the attention of interested candidates to an open postdoctoral position in my research group. Our group is currently engaged in theoretical work on coherent control of molecular processes, light-matter interactions, semiclassical methods of propagation, quantum and classical analyses of laser induced intramolecular energy redistribution, classical-quantum correspondence, quantum chaos, and decoherence. At present postdoctoral applicants are being sought to enhance our programs in coherent control and in quantum chaos. Interested applicants must be recent Ph.D. recipients and should have high quality training in either molecule-light interactions or quantum chaos/nonlinear dynamics.

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

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

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

#### **POSTDOCTORAL RESEARCH FELLOWSHIP, University of Coimbra**

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

Professor A.J.C. Varandas  
Departamento de Química

Universidade de Coimbra  
3049 Coimbra Codex, Portugal

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

#### **POSTDOCTORAL POSITION, Lawrence Livermore National Laboratory**

Two postdoctoral positions from citizens of the U.S. and NATO countries only are currently available within the Energetic Materials Center at Lawrence Livermore National Laboratory. The first position is in electronic structure theory, involving calculations of the ground and electronically excited states properties of moderate to large size energetic molecules. Experience with standard electronic structure methods (ab initio and DFT) is required, as is some programming experience. Knowledge of nonadiabatic chemistry is also helpful. The second position is at the interface of chemistry and materials science. Experience in molecular dynamics simulations is essential. Familiarity with multiscale modeling (ab initio, semiclassical and continuum modeling) is highly desirable. Qualified applicants for the two positions should submit a complete C.V. with the names and addresses of at least two references (preferably via email) to:

M. Riad Manaa, Lawrence Livermore National Laboratory, 7000 East Avenue , P. O. Box 808, L-282, Livermore, CA 94551

Fax: (925) 424 - 3281, Email: MANAA1@LLNL.GOV

#### **POST DOCTORAL POSITION, UNIVERSITY OF BORDEAUX, FR**

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

#### **POSTDOCTORAL POSITION IN MOLECULAR LASER SPECTROSCOPY, Mississippi State University**

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

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

The associate can expect a salary of ~\$30-32K per year, plus medical insurance and moving expenses. Interested individuals with appropriate research background should promptly send a cover letter and a CV (preferably by e-mail or fax) and have 2-3 recommendation letters sent directly to: Dr. R. Vasudev, Mississippi State University, Diagnostic Instrumentation & Analysis Laboratory, 205 Research Boulevard, Research & Technology Park, Starkville, MS 39759-9734; Fax:(601)-325-8465; E-mail: vasudev@dial.msstate.edu.

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

We are an equal opportunity, affirmative action institution.

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

### **POSTDOCTORAL POSITION ON SINGLE MOLECULE FLUORESCENCE MICROSCOPY, University of Cambridge**

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

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

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

Bioimaging with Ultrafast Lasers

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

The post is available immediately for a period of three years

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

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

**Postdoctoral Position in Atmospheric Chemical Kinetics, University of Michigan** A postdoctoral position is available immediately to study the theory of vibrational energy transfer involving small and mid-sized molecules. A major objective is to calculate state-to-state vibrational energy transfer rate constants for use in understanding non-equilibrium effects in Earth's upper atmosphere. A second major objective is to extend the calculations to mid-size molecules with higher densities of states. A suite of theoretical

techniques will be investigated, possibly including classical trajectories, VCC-IOS, and forced-oscillator methods. The project is a collaboration among J. R. Barker (University of Michigan), M. G. Mlynczak (NASA/Langley), and L. L. Lohr (University of Michigan). The position is available immediately (at the University of Michigan) and is for one year with extensions (by mutual agreement) for two more years. The annual salary will be 31K – 34K, depending on experience and qualifications. Preference will be given to applicants with a strong background in semi-classical and/or quantum scattering methods. Applicants should send (via e-mail or regular post) a CV and publication list, a letter describing research interests, and the names of two references to Prof. John R. Barker (jrbarker@umich.edu); Department of Atmospheric, Oceanic, and Space Sciences; The University of Michigan; Ann Arbor, MI 48109-2143. John R. Barker Department of Atmospheric, Oceanic, & Space Sciences & Department of Chemistry, 1520 Space Research Building, University of Michigan, 2455 Hayward Street, Ann Arbor, MI 48109-2143 (USA) Tel: 734-763-6239, Fax: 734-764-5137, jrbarker@umich.edu

### **POSTDOCTORAL APPOINTMENT, Argonne National Laboratory**

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

The Chemical Dynamics Program at Argonne consists of ten permanent staff members, five theoreticians and five experimentalists. It offers a unique opportunity for the close interaction between theory and experiment. The group has a leadership role in a network of groups at Argonne that have a common interest in the simulation of combustion systems. The postdoctoral appointment will carry out research in the context of this network. In this regard, joint projects with computational fluid dynamicists from other groups involved in direct numerical simulation of combustion processes may arise during the course of this appointment. The position is available immediately. Applicants must have received their Ph.D. no later than three years before their starting date.

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

Please send a c.v. and have two letters of recommendation to: Albert Wagner or Michael Davis, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439

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

### **POSTDOCTORAL POSITION, University of Waterloo**

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

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

The Atmospheric Research Group at the University of Waterloo is a collaboration between Prof. J. Pawliszyn and Prof. J.J. Sloan. Presently, it is focused on the development of new monitoring techniques for tropospheric gas phase and particulate pollutants, with a strong emphasis on urban and indoor air quality.

The successful candidate will lead the expansion of this group into the area of modelling. There will be substantial assistance from our collaborators in government and private industry with this effort. Further information about related experimental projects in the Atmospheric Research Group may be found at our website: <http://www.science.uwaterloo.ca/chemistr/>, where the individual pages may be found at [pawliszyn.html](#) and [sloan.html](#).

The University of Waterloo, which has approximately 20,000 students, is located in Waterloo, Ontario, 100 km west of Toronto. The Kitchener-Waterloo urban area has a population of approximately 250,000, and is surrounded by a pleasant, mostly agricultural, rural region.

Applicants should forward a CV and two letters of reference to: Prof. J.J. Sloan, Departments of Chemistry and Physics, University of Waterloo, Waterloo ON N2L 3G1, Canada. Tel: 1 519 888 4401, Fax: 1 519 746 0435, e-mail: [sloanj@UWaterloo.CA](mailto:sloanj@UWaterloo.CA)

### **POSTDOCTORAL POSITION, Weizmann Institute of Science, Israel**

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

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

### **POSTDOCTORAL POSITION, National Taiwan University**

A postdoctoral position is currently available in the Department of Chemistry, National Taiwan University, Taipei, Taiwan. The research will focus on one of the two topics: 1. photodissociation and photoionization of van der Waals molecules using a reflectron time-of-flight MS and 2. ion-molecule reactions using a new apparatus which is being constructed. Therefore, a candidate should have experience with pulsed molecular beam, laser technique, and mass spectrometer. The initial appointment will be for one year, but funds are available for support more than one year. Applicants should send a CV and two letters of recommendation to Professor K. C. Lin, Dept. of Chemistry, National Taiwan University, Taipei, Taiwan 106, ROC. Tel: 886-2-23621483; Fax: 886-2-23621483; e-mail: [kclin@mail.ch.ntu.edu.tw](mailto:kclin@mail.ch.ntu.edu.tw).

### **POSTDOCTORAL POSITION, University of Kentucky**

One postdoctoral research associate position is available IMMEDIATELY in the area of laser spectroscopy and chemistry. The position is initially for one year and may be renewable upon the mutual agreement. The research associate will work on metal clusters and metal-ligand complexes using ZEKE spectroscopy, photoionization spectroscopy, time-of-flight mass spectrometry, and ab initio calculations. Applicants should have experience in laser spectroscopy or related areas. Persons interested are encouraged to send (preferably

by e-mail or fax) a cover letter, a CV, a list of publications, and the names and addresses of two references to: Dong-Sheng Yang, Department of Chemistry, Chemistry-Physics Building, Room 9, University of Kentucky, Lexington, KY 40506-0055.

Tel: (606) 257-4622, Fax: (606) 323-1069, E-mail: dyang0@pop.uky.edu

URL: <http://www.chem.uky.edu/research/yang/>

Applications will be considered until the position is filled. The University of Kentucky is an EO/AA employer.

#### **POSTDOCTORAL POSITION, University of Queensland, Australia**

Postdoctoral positions are available immediately in the Computational Reaction Dynamics Group lead by Dr Sean Smith at the University of Queensland, Brisbane, Australia. The position will be offered initially for one year, with the possibility of extension beyond that subject to mutual satisfaction. The work will focus on the development of iterative quantum scattering methodologies for application to unimolecular dissociation and collision-complex-forming bimolecular reactions. Salary negotiable, dependent on the qualifications of the applicant. A summary of the theoretical activities in our group and recent publications can be accessed via my webpage.

A postdoctoral position in the area of theoretical/computational reaction kinetics is available immediately in the Computational Reaction Dynamics Group (CRDG) at the University of Queensland. The successful candidate will be involved in applying any or all of

(1) microcanonical variational transition state theory (generalised reaction coordinate), (2) classical trajectories, (3) electronic structure calculations and (4) stochastic master equation solutions for the modelling of fast radical + unsaturated hydrocarbon reactions of importance in combustion, atmospheric and interstellar chemistry. This work will form part of a collaborative initiative between the CRDG at University of Queensland (<http://www.chemistry.uq.edu.au/homepages/crdgroup/>) and the Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica, Taiwan, where these reactions are being studied experimentally in a crossed-molecular-beam apparatus (<http://po.iams.sinica.edu.tw/~kaiser/>). Interested candidates are invited to send (electronically) a resume and the names of two potential referees to myself, address as below.

Sean C. Smith, Senior Lecturer, Department of Chemistry, University of Queensland, Qld 4072, Brisbane, Australia.

tel (617) 33653975, fax (617) 33654299, email: s.smith@chemistry.uq.edu.au

Web: <http://www.chemistry.uq.edu.au/homepages/smith/index.html>

#### **POSTDOCTORAL POSITION, University of California, Berkeley**

A postdoctoral position is available immediately in the research group of William A. Lester, Jr., University of California, Berkeley. The research is focused on theoretical studies of reaction pathways and molecular properties using quantum Monte Carlo and other ab initio electronic structure methods. Applicants with strong backgrounds in electronic structure methods including effective core potentials and code development will be given preference. Please send CV listing experience, publications, and presentations as well as the names, telephone and fax numbers, and e-mail addresses of two references to the address below. In addition, please request references to forward letters to the following address.

Professor William A. Lester, Jr., Department of Chemistry, University of California, Berkeley, Berkeley, CA 94720-1460, U.S.A.

Tel: (510) 643-9590; Fax: (510) 486-5574; Homepage:<http://www.cchem.berkeley.edu/~walgrp/>

#### **SCIENTIST, University of Waterloo, Canada**

The candidate will supervise reduction and analysis of data from the ACE (Atmospheric Chemistry Experiment) satellite to be launched in 2001, in collaboration with members of the ACE Science Team at the University of Waterloo. The ACE mission is funded by the Canadian Space Agency for a 5-year period,

1999-2003. The ACE instrument is a high-resolution infrared Fourier transform spectrometer that will measure atmospheric absorption spectra by solar occultation. The job responsibilities will include ensuring the orderly flow of data, and data integrity as well as the development and improvement of the data handling software. Experience with Fourier transform spectroscopy and atmospheric chemistry is required. In addition, direct experience with satellite data processing would be a substantial advantage. The candidate will have the opportunity to participate in the scientific publications arising from the measurements and to co-supervise graduate students and post-doctoral fellows in the research groups at Waterloo.

To apply, send a c.v. and the names of three references to: Peter Bernath, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1  
telephone: 519-888-4814, fax: 519-746-0435, email: bernath@uwaterloo.ca

#### **POSTDOCTORAL POSITION, Carnegie Mellon University**

A postdoctoral position in experimental physical and biophysical chemistry is now available with Professor Linda Peteanu in the Department of Chemistry at Carnegie Mellon University. The successful candidate will participate in experiments examining the effect of molecular environment on charge-transfer reactions using Stark, fluorescence, and resonance Raman spectroscopies. The focus of the research is the photochemistry and photophysics of retinals and other polar donor-acceptor polyenes in glassy and polymeric matrices. Opportunities to study charge-transfer reactions in proteins and in organic compounds, conducting polymers, and to participate in the development of novel spectroscopic methods will also be available to the successful applicant. A Ph.D. is required, preferably in physical chemistry, physical organic chemistry, or biophysical chemistry. Additional preference will be given to candidates who have experience with laser spectroscopy and/or familiarity with the synthesis, isolation and characterization of organic compounds. Experience working with biological materials and with computational chemistry programs is also useful. The position is initially for one year but may be extended for an additional year by mutual consent. The salary is negotiable. Interested candidates should send a cover letter, a curriculum vitae, and have three letters of recommendation sent directly from the referees to:

Professor Linda Peteanu, Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, PA 15213 USA  
phone: 412-268-1327, fax: 412-268-6897, email: peteanu@andrew.cmu.edu

#### **POSTDOCTORAL POSITION, Weizmann Institute**

2 post-doctoral positions in the fields of theoretical and experimental "Coherent Control" have become available in the group of Moshe Shapiro at the Weizmann Institute of Science, Rehovot, Israel.

The experimental work will focus on 2-photon vs. 2-photon phase control of dissociation processes, in continuation of our past demonstration of laser control of electronic degrees of freedom in the Na<sub>2</sub> dissociation process (Phys. Rev. Letters 76: 2886 (1996)).

The theoretical work will deal with: coherent control of chiral synthesis; laser cooling of molecules and laser induced recombination; wavepacket and potential imaging by femtosecond spectroscopy.

Additional details about the group, its activities, and two sample papers, can be found at <http://chemphys.weizmann.ac.il/~shapiro/home.html>

Interested applicants should contact (electronic mail is preferable):

Professor Moshe Shapiro, Department of Chemical Physics, The Weizmann Institute, Rehovot, 76100, Israel  
fax: +972-8-9344123, cfshapir@weizmann.weizmann.ac.il

#### **POSTDOCTORAL POSITION, University of Notre Dame**

Applications are invited for a POSTDOCTORAL POSITION in experimental gas/surface reaction dynamics at the University of Notre Dame. Reactions between incident ions and surface adsorbates are explored under UHV conditions. Ions are accelerated to hyperthermal energies (5-300 eV) and collide with well-characterized single-crystal surfaces. A differentially-pumped QMS is used to detect scattered products

with angular-, mass-, and energy-resolution. In addition, TPD, AES, XPS, and Kelvin Probe measurements are employed to monitor surface modifications following prolonged ion beam exposures. The mechanisms for charge transfer, dissociation, and atom abstraction reactions are probed by measuring how the reaction probability and product distributions depend on the collision energy, angle-of-incidence, and the surface adsorbate structure. Candidates with previous experience in charged particle optics and/or surface science techniques are especially encouraged to apply. Applicants should send a curriculum vitae and arrange for two letters of recommendation to be sent to:

Prof. Dennis C. Jacobs, Dept. of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, USA

Phone: (219)631-8023, FAX: (219)631-6652, Home Page - <http://www.nd.edu/~djacobs>

### **POSTDOCTORAL POSITION, University of Osnabrueck**

A postdoctoral position (BAT IIa) is available in the field of aerosol physics at the Department of Physics of the University of Osnabrueck for three years with special emphasis on physical and chemical properties of levitated aerosols.

This project is primarily focused on laboratory experiments on the characterization of physical and chemical properties of single levitated aerosol particles of tropospheric and stratospheric relevance. Chemical transformations of atmospheric trace gases occurring on aerosol particles will also be investigated. The particles are stored in electrodynamic traps. Methods for in situ- and ex situ-characterization of the aerosols include: elastic and inelastic light scattering, optical spectroscopy, and mass spectrometry.

Applicants should have experience in the above mentioned fields. They should also be motivated to participate in interdisciplinary collaboration projects in environmental research. Applicants are required to assist in teaching of students and they should have a diploma or equivalent degree in physics or chemistry as well as a Ph.D. in physics or physical chemistry. The position is suitable for further qualification. There is the possibility of part-time work.

The University of Osnabrueck endeavors to employ a higher portion of female academic staff. Female candidates are therefore encouraged to apply, and will be selected if suitably qualified. Physically handicapped applicants will take precedence if equally qualified.

Applications containing the customary documents should be sent by 01.05.99 to the Dekan des Fachbereichs Physik, Universitat Osnabrueck, Barbarastr. 7, D-49069 Osnabrueck, Germany.

### **POSTDOCTORAL POSITIONS, Georgia Institute of Technology**

Two postdoctoral research positions are available in the group of Prof. Rigoberto Hernandez at the Georgia Institute of Technology with starting dates between September 1, 1999 and February 1, 2000.

I. One opening will be involved with further developing iGLE and WiGLE – an irreversible nonequilibrium stochastic dynamics – and its application to polymerization processes. This NSF-funded work will involve collaboration with a former postdoctoral student, Frank Somer, who will be starting a tenure-track position at St. John's University in fall '99. See, e.g., Hernandez and Somer, *J.Phys.Chem.B* V.103, 1064 and 1070 (1999).

II. One opening will be involved with the development and study of dynamic models describing protein folding. This work will involve collaboration with a graduate student. A publication analyzing some interesting features of minimalist models is currently in preparation.

Both positions are for a two year tenure (one year, renewable for second year), and will be compensated by a generous salary (proportional to experience) and health benefits. Interested individuals should send a statement of research interests, a Curriculum Vitae and the names of three references by e-mail to [jhernandez@chemistry.gatech.edu](mailto:jhernandez@chemistry.gatech.edu), or by regular post.

Rigoberto Hernandez, Blanchard Assistant Professor of Chemistry, School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400 USA.

FAX: (404) 894-7452, E-Mail: hernandez@chemistry.gatech.edu

Web site: <http://www.chemistry.gatech.edu/rig>

### **POSTDOCTORAL POSITION, Argonne National Laboratory**

The Gas Phase Chemical Dynamics Program at Argonne National Laboratory has an opening for a post doctoral appointment working with R. Glen Macdonald. The research involves the use of high resolution time-resolved near infrared and infrared absorption spectroscopy to study the spectroscopy, dynamics and kinetics of radicals of interest to combustion and atmospheric chemistry. The main thrust of the program over the next few years will be to study the dynamics and kinetics of atom + radical and radical + radical processes; however, other studies are possible, depending on the qualifications and interests of the successful candidate. Several recent articles will give potential candidates an idea of the variety of problems that can be tackled with this apparatus; a) Infrared Spectroscopy, *J. Mol. Spectroscopy* 186, 349 (1997). b) Chemical Kinetics, *J. Phys. Chem.* 102, 4585 (1998), and c) Chemical Dynamics, *J. Chem. Phys.* 109, 4224 (1998). The successful candidate should be planning to graduate soon or be a recent graduate from a Chemical Dynamics or Kinetics Program (within the last 3 years), and have experience in laser spectroscopy, vacuum techniques, and computer data acquisition. A background in rovibrational spectroscopy of polyatomic molecules would be a desirable asset. An application will require a CV and three letters of recommendation. For further information, interested candidates should contact Glen Macdonald.

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

R. Glen Macdonald, Argonne National Laboratory, Chemistry Division, 9700 South Cass Ave., Argonne, IL 60439

Ph:(630) 252-7742, Fax:(630) 252-4470, Email: macdonald@anlchm.chm.anl.gov

### **POSTDOCTORAL POSITION, Sandia National Laboratories**

A Post-Doctoral Position is available at Sandia National Laboratories in Livermore, California. The Combustion Research Facility is seeking a recent PhD scientist or engineer interested in MOLECULAR SENSOR DEVELOPMENT and applications. The successful candidate will join a team that is actively developing and applying optical spectroscopic techniques for real-time sensors of interest to the Departments of Energy, Defense, and U.S. industry. Current work has been based on tunable-diode-laser ABSORPTION SPECTROSCOPY in the mid- and near-infrared regions, and new laser-based mid-infrared sources are being developed in conjunction with other teams at Sandia. Many of the sensor applications are in highly particle-laden gas streams at high temperature. An example of current activities is the application of time-resolved measurements of gas-phase concentrations and temperatures for real-time control of processes in both basic oxygen and electric arc steelmaking. In addition to commercial steelmaking, we are currently conducting experiments in demilitarization of conventional munitions, large-scale pool fires, and the assessment of long-term aging of organic materials in weapons components. The successful candidate will be exceptionally strong technically and be a creative problem-solver. Candidates should have a Ph.D. in either the physical sciences or engineering and have demonstrated experimental and modeling research experience with aspects of molecular spectroscopy, optics, lasers, combustion diagnostics, electronics, computer simulation, data analysis and methods for process control. Experience with fiber-optically coupled lasers is also advantageous. Laboratory and communications skills must be excellent, and the ability to work independently or in a team environment is a must. Travel for field experiments is required for this position. Please send a resume, with names of references, statement of research expertise, and copies of college transcripts to:

Sandia National Laboratories, Anna Isham, MS 9111, HR Dept-CA0022, Job Code DRH-1250, P.O Box 969, Livermore, CA 94551-0969.

US citizenship is required. Sandia National Laboratories is an Equal Opportunity / Affirmative Action employer. For more information, please contact Sarah Allendorf, Principal Member of the Technical Staff, Sandia National Laboratories, MS 9052, P.O. Box 969, Livermore, CA 94551-0969.

Fax:(925)294-3379, email: SWALLEN@SANDIA.GOV

### **POSTDOCTORAL POSITION, University of Southampton**

Laser Driven Scanning Tunnelling Microscopy will be developed to record IR vibrational spectra of surface species with molecular spatial resolution under a £460,000 grant from the EPSRC (Chemistry & Physics programmes). The combination of a tuneable ps IR laser/OPO with a UHV STM will revolutionize surface studies by combining direct imaging and spectroscopic identification. Extensive refurbishment of the physical chemistry area is taking place and this together with a specific grant from the Wolfson Foundation will provide a purpose built area for the equipment.

We seek to appoint a PDRA with experience with either STM or laser/OPO systems, initially for one year (up to point 4, £15,753 pa) with extension possible for further years.

For further information please contact: Dr. J.G. Frey, Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, Email: j.g.frey@soton.ac.uk

Professor Brian Hayden, Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, Email: b.e.hayden@soton.ac.uk

Dr. W.S. Brocklesby, OptoElectronics Research Centre, University of Southampton, Southampton, SO17 1BJ, Email: wsb@orc.soton.ac.uk

### **POSTDOCTORAL POSITION, Columbia University**

We are searching for post-doctoral candidates to do interdisciplinary work at Columbia University in physical chemistry projects for two areas: basic studies of environmentally related surface chemistry on model metal oxide surfaces, and in the chemical physics of reaction dynamics on semiconductor surfaces. The candidates should have a strong experimental background in state-resolved laser techniques and/or in surface science. The work, which is focused by major new NSF centers in 1) environmental chemistry and 2) advanced material research, and would involve collaborative research among several research groups at Columbia. Please fax or mail your resumes including the names of three senior faculty scientists familiar with your capabilities to Prof. Richard M. Osgood, Jr. at the Columbia Radiation Laboratory, 530 West 120th Street, rm. 1001, New York, NY 10027. Fax 212-854-1909. Columbia University is an equal opportunity employer.

### **POSTDOCTORAL POSITION, University of Montreal**

I am looking for a postdoctoral fellow to work with my group at the University of Montreal, Canada. People who applied a few months ago are welcome to apply again.

The initial appointment will be for one year but funds are available for a second year. Candidates should have training in either theoretical chemistry or theoretical physics. Experience in quantum dynamics calculations would be an asset.

The group is interested in developing and applying new methods for calculating: (i) vibrational and ro-vibrational energy levels of small polyatomic molecules (JCP 99 8519 (1993), JCP 100 6175 (1994), JCP 101 8494 (1994), JCP 103 5600 (1995), JCP 107 9493 (1997), Chem Phys Lett 287 289 (1998)); (ii) rate constants (Chem Phys Lett 267 417 (1997), Chem Phys Lett 293 209 (1998)), and (iii) photodissociation cross sections (JCP 105 141 (1996)).

Interested candidates should send a C.V. and a summary of research interests to Tucker Carrington at the address below.

Tucker Carrington Jr., Departement de chimie, Universite de Montreal, Case postale 6128, succursale Centre-ville, Montreal (Quebec) H3C 3J7, Canada

tel: (514) 343-2123, fax: (514) 343-7586, e-mail: Tucker.Carrington@umontreal.ca

### **POSTDOCTORAL POSITION, University of Notre Dame**

A postdoctoral position is available in my group at the University of Notre Dame starting September 1, 1999. The position will be in the area of: Investigating small molecule diffusion through biological membranes using novel methods for molecular dynamics.

This project involves a combination of computational methods development and applications. Computer programming experience and a strong background in physical chemistry and/or chemical physics are required, although talented applicants with different backgrounds will also be considered. The exact starting date is flexible. The position will be for one year with the expectation of renewal for a second year upon mutual agreement.

Interested individuals should send a Curriculum Vitae, a statement of research interests, and at least 2 letters of recommendation to me at my current address.

Dr. J. Daniel Gezelter, Department of Chemistry, Columbia University, 3000 Broadway, Mail Code 3159, New York, NY 10027

Phone: (212) 854-5650, gezelter@chem.columbia.edu

[www.chem.columbia.edu/~gezelter](http://www.chem.columbia.edu/~gezelter)

### **POSTDOCTORAL POSITION, Marquette University**

#### **POSTDOCTORAL POSITION IN EXPERIMENTAL CHEMICAL PHYSICS**

A post-doctoral position in experimental chemical physics is available immediately in the laboratory of Scott Reid in the Department of Chemistry at Marquette University. The successful candidate will participate in experiments on the spectroscopy of jet-cooled radicals using nonlinear four wave mixing and transient grating techniques [see, e.g., JCP 110, 5734-5744 (1999)] as well as linear techniques such as cavity ring down spectroscopy and resonant photoionization. In addition, the candidate will have some opportunity to work on a second project involving the growth of new thin film materials using pulsed laser deposition and the characterization of pulsed laser desorption/ablation from solid targets using time-of-flight mass spectrometry and spectroscopic techniques [see, e.g., CPL 301, 517-523 (1999)].

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 competitive and negotiable, and initial appointment will be for one year, with an extension of one or more years by mutual consent. Interested applicants should send a curriculum vitae and have two letters of reference sent directly to:

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

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

Additional information may be found on our webpage at:

[www.mu.edu/dept/chem/faculty/html/reid.html](http://www.mu.edu/dept/chem/faculty/html/reid.html)

Marquette University is an AA/EO employer.

### **POSTDOCTORAL POSITION, Columbia University**

A postdoctoral position in the area of state-to-state dynamics of chemical reactions is available immediately in the laboratory of Professor James J. Valentini. The emphasis of the project is on the elucidation of the influence of "many-body" effects—those features that distinguish reactions in which one or both reactants are polyatomic from the prototype atom + diatom reactions. Current target systems are atom + polyatom reactions like  $H + CH_4$  and  $H + CHCl_3$  as well as more complex systems. The experiments rely on REMPI measurements—Doppler-resolved and distance-of flight/position-resolved—to map the energy distributions of both reaction products. Stimulated Raman excitation methods are used to vibrationally prepare the reactant molecule, and laser photolysis creates the reactant atom. Related studies focus on reactions in molecular

clusters, where the "many-body" effects are solvation-like. The experiments are complemented by computational simulations of the dynamics of the reactions on realistic model potential energy surfaces as an aid to interpreting the experimental results.

Interested applicants should contact Professor Valentini via email, fax, or mail, and arrange to have two letters of recommendation sent to him. The position will remain open until a suitable candidate is found. Professor James J. Valentini, Department of Chemistry, Columbia University, Mail Code 3120, 3000 Broadway, New York, NY 10027  
Phone: 212-854-7590, Fax: 212-932-1289

#### **POSTDOCTORAL POSITION, Wayne State University**

A postdoctoral position in theoretical quantum chemical dynamics is available immediately at Wayne State University in my research group. One focus of the research is the exploitation of scalable parallel computing in quantum wavepacket dynamics in order to extend the size and complexity of the systems that can be studied accurately. Parallel algorithms will be developed, implemented and applied to several interesting and computationally challenging chemical systems. One project involves further development of an efficient scalable quantum dynamics code for four atom systems and its application to several diatom-diatom and atom-triatom reactions. Another project is the use of reduced-dimensionality quantum dynamics models to study the mechanisms of organic reactions involving diradical intermediates. A list of relevant publications can be found at <http://dynamo.chem.wayne.edu/evi/publications/pub.html>.

The Chemistry department at WSU has a strong and prominent contingent of theoretical/computational chemists. Information about the chemistry department can be found at <http://www.chem.wayne.edu>.

This is a one year appointment with a possible renewal for a second year. Applications must have a Ph.D. in chemistry, physics or a related field. Experience with some aspect of chemical reaction dynamics and a strong background in scientific computing are highly desirable.

Interested candidates should send a CV, a publication list and three letters of recommendation to Evelyn Goldfield, Dept. of Chemistry, Wayne State University, Detroit, MI 48202, USA. It is fine to contact me directly by sending email to [evi@sun.science.wayne.edu](mailto:evi@sun.science.wayne.edu) or phone me at 313-577-2580. My fax number is 313-577-2554. Further information about Wayne State University can be found on the world wide web at <http://www.wayne.edu/>

WSU is an EO/AA educator and employer. Women and minorities are encouraged to apply.

#### **POSTDOCTORAL POSITIONS, University of California, Davis**

I have THREE postdoctoral positions coming available immediately in Theoretical and Computational Studies of Reaction Dynamics in Condensed Phases (primarily in supercritical fluids). I would appreciate if you could bring the announcement, found at

<http://www-chem.ucdavis.edu/people/tucker.html>

to the attention of any qualified and interested candidates.

Susan C. Tucker, Associate Professor, Department of Chemistry, University of California, Davis, CA 95616  
phone: 530-752-2203, fax: 530-752-8995, email: [sctucker@ucdavis.edu](mailto:sctucker@ucdavis.edu)

#### **POSTDOCTORAL POSITION, Argonne National Laboratory**

A postdoctoral position in experimental chemical physics is available starting Summer 1999 in the Metal Cluster Chemistry Group at Argonne National Laboratory (USA). Our group has initiated a new project aimed at building up an RF quadrupole ion trap (Paul trap) apparatus for the study of metal clusters and nanocrystals. We specifically invite applications from candidates who have experience in the design, construction and operation of ion traps. A background in experimental cluster chemistry/physics is also desirable, but not essential. Applicants need not be US citizens. Salary depends on experience, but starts at approximately USD 41,500. The appointment is for one to two years. Applicants should send a curriculum vitae to Mark Knickelbein at [knickelbein@anl.gov](mailto:knickelbein@anl.gov). Argonne National Laboratory is an Equal Opportunity

Affirmative Action Employer.

### **POSTDOCTORAL POSITION, CAMBRIDGE UNIVERSITY**

This position, funded by Schlumberger Cambridge Research and the Isaac Newton Trust, is available at the Cambridge University Centre for Computational Chemistry (CUC3) from October 1, 1999. The successful candidate is expected to work in close collaboration with members of CUC3 in at least one of the following areas of research : - DFT of electronic structure - Theory of intermolecular forces - Ab initio (Car-Parrinello) simulation of aqueous chemistry and materials - Statistical Mechanics and simulation of clusters, complex fluids, glasses and proteins. Extensive knowledge of advanced numerical and simulation techniques is essential.

The appointment is for an initial period of three years, renewable for a further two years, and will be on the University's standard scale in the range 15,735 to 23,651 pounds sterling (currently under review), according to age and experience. Applications (in duplicate) including a CV and the names and addresses of two referees should be sent to Professor J. P. Hansen, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW to arrive not later than August 1, 1999.

For further information see <http://www.ch.cam.ac.uk/>

### **POSTDOCTORAL POSITION, UNIVERSITY OF AKRON**

Continuous-wave cavity ringdown spectroscopy is a high sensitivity method for recording fully resolved infrared spectra. Our objective is to obtain precise information about torsion-vibration and vibration-vibration coupling pathways important in intramolecular vibrational redistribution (IVR) in small molecules. Methanol was chosen for study because it is becoming a benchmark system for studies of IVR and because of its relevance to combustion systems. The work is funded by the U.S. Department of Energy. Additional information on the University of Akron Department of Chemistry and the Perry research group may be found on the web at <http://www.chemistry.uakron.edu>.

The postdoctoral fellow's primary work will be implementation and application of the cavity ringdown technique. In addition, the fellow will be involved in the analysis of and quantum mechanical modeling of high resolution spectra. There is also the possibility of participation in the collaboration with T. R. Rizzo's group in the EPFL in Lausanne, Switzerland. A funded NSF International Programs grant enables collaborators from Akron to spend 3 month periods doing IRLAPS (infrared laser-assisted photodissociation spectroscopy) experiments in Lausanne. Together, the rotationally resolved experiments in Akron and Lausanne span the frequency range from 2900 to 25,000  $\text{cm}^{-1}$  and probe IVR timescales from 100 fs to 1 ns. The successful candidate will be highly motivated toward a successful research career and will have demonstrated research productivity. A Ph.D. degree in chemistry, physics, or a related area is expected. Skills with lasers, optics, electronics, vacuum systems, and computers are needed for this position.

An initial appointment will be for 1 year at a salary commensurate with experience and qualifications. Funding is available for a second year and renewal will be by mutual agreement. Applications may be sent by email or regular mail to Professor David S. Perry, Department of Chemistry, University of Akron, Akron, OH 44325-3601.

Phone: 330-972-6825, Fax: 330-972-7370, Email: [Dperry@UAkron.edu](mailto:Dperry@UAkron.edu),

Include a C.V., a description of research skills, and arrange for at least two letters of recommendation to be sent. The University of Akron is an equal opportunity/affirmative action employer.

### **POSTDOCTORAL POSITION, UNIVERSITY COLLEGE LONDON**

Applications are invited for a postdoctoral position in the Department of Chemistry at University College London in Dr. David Rowley's research group. The project, sponsored by the U.K. Natural Environment Research Council, involves the laboratory study of kinetics and mechanisms of gas phase peroxy radical reactions. These studies will be carried out in collaboration with theoretical studies of peroxy radical reactions led by Professor David Clary, and atmospheric modelling studies incorporating the laboratory data

are planned.

Interested candidates should contact Dr. David Rowley for further details before applying. The position is initially for 1 year, expected to commence in autumn 1999.

Further details of current research interests may be found at

<http://calcium.chem.ucl.ac.uk/webstuff/people/rowley/>

Dr. David M. Rowley, University College London, Chemistry Department, Christopher Ingold Laboratories, 20 Gordon Street, London WC1H 0AJ, United Kingdom

Tel 0171 504 4775, International +44 171 504 4775 Fax 0171 380 7463, International +44 171 380 7463

### **POSTDOCTORAL POSITION, UNIVERSITY OF BIRMINGHAM**

Applications are invited for a postdoctoral fellowship in astrophysical chemistry under the supervision of Professor Ian WM Smith and Dr Ian R Sims, and funded by the European Union's TMR Programme, as part of the TMR Network on "Astrophysical Chemistry: Experiments, Calculations, and Astrophysical Consequences of Reactions at Low Temperatures."

Experiments are planned to investigate reaction kinetics and dynamics, and energy transfer processes relevant to the interstellar medium at temperatures as low as 7 K, using lasers coupled to a novel supersonic flow technique. More details of the research field and the techniques used may be found at the following sites:

[http://web.bham.ac.uk/i.r.sims/irsims/sims\\_res03.html](http://web.bham.ac.uk/i.r.sims/irsims/sims_res03.html)

[http://web.bham.ac.uk/i.r.sims/irsims/sims\\_res04.html](http://web.bham.ac.uk/i.r.sims/irsims/sims_res04.html)

and details of the Astrophysical Chemistry TMR Network should also be consulted:

<http://www.bham.ac.uk/Astrochemistry/>

The position is available from September 1999 for two years (one year renewable for a further year). The exact commencement date is negotiable. Under the terms of the TMR Programme, applicants must be nationals of a Community Member State or a State associated with the TMR Programme (Iceland, Israel, Liechtenstein, Norway). The young researchers must not be nationals of the state in which the participant appointing them is established (i.e., the UK) and must not have carried out their normal activities in that state for more than 18 of the 24 months prior to their appointment. Please follow the link below for full details on eligibility conditions:

<http://www.cordis.lu/tmr/src/elcond.htm>

Informal enquiries can be made to Dr Ian R Sims, School of Chemistry, The University of Birmingham, Edgbaston, Birmingham, B15 2TT UK

Tel: +44 121 414 3782, Fax: +44 121 414 4426, Email: [i.r.sims@bham.ac.uk](mailto:i.r.sims@bham.ac.uk)

or

Professor Ian W.M. Smith FRS at the School of Chemistry Tel: +44 121 414 4422; fax: +44 121 414 4426; E-mail: [i.w.m.smith@bham.ac.uk](mailto:i.w.m.smith@bham.ac.uk)

### **POSTDOCTORAL POSITION, UNIVERSITY OF YORK**

Applications are invited for a Postdoctoral Fellowship, tenable for up to 4 years. The successful applicant will play a key role in a project to build a new instrument for characterisation of biomolecules with laser induced evaporation. Informal enquiries may be made to Professor Klaus Mueller-Dethlefs (Tel: 01904 434526; email: [kmd6@york.ac.uk](mailto:kmd6@york.ac.uk)).

The research fellowship is associated with a project funded under the EPSRC instrument development programme to build a new instrument for the characterisation of biomolecules with laser induced evaporation. The proposed instrument will incorporate two different types of laser desorption sources; one employing laser desorption from a rotating rod and the other laser induced liquid beam ionisation/desorption which uniquely allows desorption of biomolecules without denaturation. Characterisation of the biomolecules will be achieved with laser photoionisation time-of-flight mass spectrometry and photoelectron spectroscopy. Interested candidates should ideally have experience with instrumentation and lasers and a

strong interest in spectroscopy and biomolecular chemistry and/or physics, although the latter is not essential. Salary in the range £15,735 - £18,275 per annum, within Grade IA of the scales for research staff. Further particulars and details of how to apply may be obtained by writing to the Personnel Office, University of York, Heslington, YORK YO10 5DD or by email on jobs@york.ac.uk, quoting reference number /6034. The closing date for applications is Friday 9 July 1999.

Professor Klaus Mueller-Dethlefs, Chair of Physical Chemistry, Department of Chemistry, The University of York, York YO10 5DD, United Kingdom

Tel: +44 1904 434526, Direct Fax: +44 1904 434527, Secr Tel: +44 1904 432525, Dept Fax: +44 1904 432516

### **POSTDOCTORAL POSITION, BEN-GURION UNIVERSITY**

Applications are invited for an open postdoctoral position in the research group of Professor S. Rosenwaks and Dr. I. Bar. Our group is currently engaged in experimental work on exploration of ground and excited state intramolecular dynamics utilizing vibrationally and rovibrationally mediated photodissociation in molecules which may reach selectivity, including molecules which are of relevance to atmospheric chemistry [JCP 107, 8476 (1997), JPC A, 102, 7273 (1998), JCP 109, 8959 (1998)]. Details can be found at [http://www.bgu.ac.il/phys/people/homepages/zamik\\_rosenwaks.html](http://www.bgu.ac.il/phys/people/homepages/zamik_rosenwaks.html) Interested applicants must be recent Ph.D. recipient and should have experience with pulsed molecular beams, lasers and time-of-flight mass spectrometry. The initial appointment will be for one year, but funds are available for longer support. Salary is ca. 22,000 USD per year, more than enough to cover living and housing expenses in Israel. Applicants are asked to send their Curriculum Vitae and should also arrange to have two or more letters of recommendation sent to Professor Rosenwaks directly, either by email or by regular mail: Professor S. Rosenwaks, Department of Physics, Ben-Gurion University of the Negev, P.O.Box 653, Beer-Sheva 84105, Israel Fax: 972-7-647-7745, Tel: 972-7-6472-421/2/3/4, Email: zamik@bgumail.bgu.ac.il

### **POSTDOCTORAL POSITIONS, UNIVERSITY OF DURHAM**

One or two postdoctoral Senior Research Assistant positions are available, to work in Prof. Jeremy Hutson's theoretical chemical physics group. The appointments will be for 1 year in the first instance, starting as soon as convenient.

Further particulars of the posts and application forms are available from the Personnel Office, University of Durham, Old Shire Hall, Old Elvet, Durham, DH1 3HP, UK, or by email from [acad-recruit@durham.ac.uk](mailto:acad-recruit@durham.ac.uk). Please quote reference A170D. Completed forms, accompanied by a full curriculum vitae and the names of two academic referees, must be received by the Personnel Office by 13 August 1999.

The Research Projects and Job Descriptions

Position 1 is for a Senior Research Assistant to work with Prof. Jeremy Hutson and Dr. Pavel Soldan on an EPSRC-funded research project entitled "Long-range interactions involving atomic and molecular ions".

The main thrust of the project is to use the spectra of near-dissociation states of ionic complexes such as  $\text{Ne}_2^+$ ,  $\text{Ar}_2^+$ ,  $\text{NeN}^+$  and  $\text{HeH}_2^+$ , which have recently been measured by Carrington and coworkers (Southampton), to learn about the potential energy surfaces for ionic interactions and the dynamics of near-dissociation states. We have used similar spectra of  $\text{HeAr}^+$  and  $\text{HeKr}^+$  to develop reliable potential surfaces (or, equivalently, sets of potential curves and the couplings between them), and have carried out high-level ab initio calculations on  $\text{He-H}_2^+$  designed to assist in assigning its spectra. See J. Chem. Phys. 102, 2379 (1995) and 105, 8602 (1996) and Chem. Phys. Lett. 260, 395 (1996) for more details.

The current project is to extend these studies to: polyatomic systems; homonuclear systems, where the  $g/u$  symmetry of the states may be broken sufficiently close to dissociation; and triplet states

An exciting recent development is the possibility of "morphing" ab initio potential energy surfaces to fit experimental data. The original potentials need not be of "spectroscopic" quality, but are "bent and stretched" to bring them into agreement with experiment. The morphing procedure offers the prospect of

obtaining potentials of "spectroscopic" quality for much larger systems than previously.

Position 2 has a wider remit. Jeremy Hutson is currently Head of the Chemistry Department, and the Department has agreed to fund a postdoctoral Research Assistant to underpin his group's research activities during his term as Chairman. The Senior Research Assistant will be expected to: Undertake research on intermolecular forces, especially on extending the "morphing" approach described above; Organise group meetings; and assist with the day-to-day supervision (and recruitment) of research students and undergraduate project students;

Assist with research grant management.

There will also be opportunities for the successful applicant to participate in making research grant proposals and to undertake some teaching duties.

Further information on the research group and the University of Durham is available at

<http://www.dur.ac.uk/~dch0www/Staff/jmh>

For both positions, the successful applicant will require either a Ph. D. or postdoctoral research experience in theoretical chemistry or chemical physics.

The salary will be on the standard RA 1A scale for research staff in UK Universities. The scale runs from 16,286 – 24,479 pounds per annum, according to age and experience, but the funding available is such that these appointments will have to be made near the lower end of the scale.

Other theoretical chemistry research groups at the University of Durham include those of: Mark R. Wilson (atomistic modelling of molecular materials), David J. Tozer (fundamental studies of density-functional theory), Stuart C. Althorpe (theory of chemical reaction dynamics).

There are also close links with the Durham Physics Department, including David Flower (molecular collisions), Robert Potvliege (multiphoton processes), Charles Adams (laser cooling and trapping), Brian Bransden (electron and positron collisions with molecules), Stewart Clark (materials modelling).

Note that Jeremy Hutson will be in the USA for almost all the period from now to the closing date, and may not be able to answer email promptly.

Prof. J. M. Hutson, Dept. of Chemistry, University of Durham, Durham, DH1 3LE, England

Tel. +44 191 374 3110 (International), FAX: +44 191 386 1127

World-Wide Web home page: <http://www.dur.ac.uk/~dch0www/Staff/jmh/>

### **POSTDOCTORAL POSITION, BEN GURION UNIVERSITY**

I have a position for a postdoctoral fellow in theoretical chemical physics. I am looking for a creative and motivated individual with experience in these or related areas, to work with me at the chemistry department in Ben Gurion-University of the Negev in Israel.

The postdoctoral fellowship is funded by the United States Israel Binational Science Foundation, through a grant to the project of "Nonclassical energy-transfer processes within a single molecule", to be conducted in Ben Gurion-University of the Negev, in a collaboration with Harvard University.

If you know of a suitable person, I would be extremely grateful if you could bring this opportunity to his/her attention.

Interested parties should send a CV and reprints or preprints of selected papers, and have at least two letters of reference sent to me at the address or email address given below.

Thank you in advance,

Bilha Segev, Department of Chemistry, Ben-Gurion University of the Negev, POB 653, Beer-Sheva 84105, ISRAEL

phone: 972-7-6472187, fax: 972-7-6472943, email: [bsegev@bgumail.bgu.ac.il](mailto:bsegev@bgumail.bgu.ac.il)

### **POSTDOCTORAL POSITION, UNIVERSITY OF BRISTOL**

A postdoctoral research assistantship in laser photochemistry is available in the group of Prof Mike Ashfold at the School of Chemistry, University of Bristol UK.

Applications are invited for a post-doctoral research assistanship funded by the Leverhulme Trust from 1 October 1999. The work will involve extension of the technique of H atom photofragment translational spectroscopy in order to:

- (1) make quantitative high resolution studies of the primary photochemistry of a range of prototypical hydrides at user selected wavelengths in the vacuum ultraviolet.
- (2) investigate the photochemistry (and thermochemistry) of jet-cooled free radical hydrides
- (3) explore the vibrationally mediated photodissociation of hydride molecules.

For recent illustrations of work under this program see: J. Chem. Phys. 110, p281 (1999), Phys. Chem. Chem. Phys. 1, p45 (1999); 1, p767 (1999) and 1, p3247 (1999).

Applicants should have a PhD in Physical Chemistry/Chemical Physics; experience with molecular beam technology, lasers and molecular spectroscopy/photochemistry would be an advantage. Starting salary will be on the RA1A scale in the range £17,238 - £19,869 per annum according to age and experience.

Further information: e-mail [mike.ashfold@bris.ac.uk](mailto:mike.ashfold@bris.ac.uk) or <http://www.jobs.ac.uk> or <http://www.chm.bris.ac.uk/pt/laser/vacancies.htm>

For further details, telephone (0117) 954 6947, minicom (0117) 928 8894 or e-mail [recruitment@bris.ac.uk](mailto:recruitment@bris.ac.uk) (stating postal address only) quoting reference 5714. Applicants will be required to send a CV and the names of two referees to the Personnel Office. Closing date: 13 August 1999.

Dr Andrew J. Orr-Ewing, School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK.

tel: +44 117 928 7672, fax: +44 117 925 1295, [a.orr-ewing@bristol.ac.uk](mailto:a.orr-ewing@bristol.ac.uk)

<http://www.bris.ac.uk/Depts/Chemistry/staff/aoewing.htm>

#### **POSTDOCTORAL POSITION, UNIVERSITY OF BRITISH COLUMBIA**

Applications are invited for a postdoctoral position in the research laboratory of Prof. Bernie Shizgal at the University of British Columbia, Vancouver, Canada. The position is available as of Sept. 1, 1999 for a recent PhD graduate with a proven expertise in kinetic theory, plasma physics and numerical methods of solution of differential equations. The research is funded by a grant directed towards the development of kinetic theory models of plasma sheaths in discharge devices. The position is initially for one year but renewal is possible. The appointment can be made either in the Department of Chemistry or the Department of Physics Those interested in the position should submit a CV, a list of research publications, and the names of three referees to;

Prof. Bernie D. Shizgal, University of British Columbia, Department of Chemistry, 2036 Main Mall, Vancouver, British Columbia V6T 1Z1, Canada

Tel: (604) 822-3997, Fax: (604) 822-2847, Email: [shizgal@theory.chem.ubc.ca](mailto:shizgal@theory.chem.ubc.ca)

<http://www.science.ubc.ca/~chem/brochure/shizgal.html>

#### **POSTDOCTORAL POSITION, UNIVERSITY OF CALIFORNIA, DAVIS**

A postdoctoral position is currently available to study the photodissociation of cometary molecules using velocity imaging. Vacuum ultraviolet light is produced by four wave mixing of ultraviolet laser light. This light is used to dissociate molecules in the VUV region that are thought to be responsible for the formation of free radicals and products in comets and planetary atmospheres. The heavy and light products are then analyzed with a second VUV laser directly in either a one-photon process or using a multiphoton scheme. The ions are imaged onto a multichannel plate detector, which produces electrons that are accelerated onto a phosphor screen. The resulting image is recorded with a camera and analyzed to determine the velocity and angular distributions.

The laboratory is well equipped for this study with two 30Hz Nd-Yag laser, 4 dye lasers, 5 excimer lasers, computers, electronics, an imaging apparatus along with a variety of other experimental systems. Experience with ultra high vacuum systems, Nd-Yag lasers and dye lasers, and mass spectrometry is desired but not

essential.

The University of California, Davis is located 60 mi. east of Berkeley, 75 east of San Francisco, and 17 mi. west of Sacramento. It is also only 125 mi. to the ski country around Lake Tahoe.

The position is for one year and is renewable for a second year. Please send a short CV along with the names of three references to: William M. Jackson, Chemistry Department, University of California, 1-Sheilds Ave., Davis, CA 95616, USA

(530) 752-6310 (Voice), (530) 752-8995 (Fax), wmjackson@ucdavis.edu

#### **POSTDOCTORAL POSITION, UNIVERSITY OF CALIFORNIA, SANTA BARBARA**

A position is available immediately for development of a new mass spectrometric approach to biopolymer analysis based on rapid evaporative cooling . Potential applications include high-speed gene sequencing and analysis of protein DNA interactions. The successful applicant will have experience with molecular beams, mass spectrometry and/or lasers. Experience in custom instrument design and construction is particularly desirable. This position is an excellent opportunity for an instrument-oriented physical chemist to branch out into problems of biological interest. This is also an opportunity to learn wet-biochemical methodology (e.g. recombinant DNA techniques). Initial appointment will be for one year with a strong likelihood of extension for a second year.

Interested applicants should send one CV with three references to:

Professors Alec Wodtke and Norbert Reich, Department of Chemistry UCSB, Santa Barbara CA 93106. Wodtke@chem.ucsb.edu, Reich@chem.ucsb.edu Fax- 1 805 893 4120

References: Rapid evaporative cooling suppresses fragmentation in mass spectrometry: Synthesis of "Unprotonated" water cluster ions., Rienk T. Jongma, Yuhui Huang, Shiming Shi, and Alec M. Wodtke, J. Phys. Chem. A102:8847-8854 (1998)

#### **POSTDOCTORAL POSITION, PENNSYLVANIA STATE UNIVERSITY**

A postdoctoral position has become immediately available in my laboratory.

Project: Spectroscopy of Molecules in Cold Helium Droplets

Nano-droplets of about 10000 helium atoms are produced in a cold molecular beam source and doped with foreign atoms or molecules. The atoms or molecules can form aggregates or react in cold collisions within the helium trap and are spectroscopically studied by using various laser techniques. Currently, high-resolution laser double resonance and resonant multiphoton ionization spectroscopy can be applied. The apparatus is complete and produces immediate results.

The investigation of doped helium nano-droplets represents an exciting new area of research. The droplets are possibly a finite-size superfluid medium. Moreover, the "helium nano-cryostats" of 0.4 Kelvin temperature offer an ideal environment for the study of 1. cold collisions, 2. cold molecular reactions, 3. large molecules with dense spectra including biologically important species, 4. the aggregation of metal atoms (preparation of nanostructures).

Applicants should have an excellent record of PhD research and have experience with molecular beams and some laser spectroscopic methods. A background in chemical physics and high-resolution molecular spectroscopy will be particularly useful. The appointment is initially for one year and can be renewed. The salary will be commensurate with qualifications. The appointment can start at any time between now and fall of 1999. Applications and two letters of recommendation should be sent to Professor Wolfgang E. Ernst, Departments of Physics and Chemistry, The Pennsylvania State University, 104 Davey Laboratory, University Park, PA 16802, USA  
or by e-mail to weel@psu.edu

#### **POSTDOCTORAL POSITION, WEIZMANN INSTITUTE, REHOVOT, ISRAEL**

A position is available in the research group of David Tannor at the Weizmann Institute, with a flexible starting date. Applicants should be 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); J. Chem. Phys. 109, 3028 (1998); J. Chem. Phys. 110, 2761 (1999); PCCP 1, 1081 (1999).) 2) Phase space approach to quantum condensed phase dynamics, (J. Chem. Phys. 107, 5236 (1997); J. Chem. Phys. 5141 (1997), J. Chem. Phys. (1999, accepted)). 3) Laser control and laser cooling of molecules, (Phys. Rev. A 56, 4929 (1997); J. Chem. Phys. 99, 196 (1993); J. Chem. Phys. 106, 1435 (1997); Faraday Disc. (1999, submitted)). 4) Dynamics of multielectron atoms (Phys. Rev. E (1999, submitted)).

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. More information, preprints and links are available at <http://chemphys.weizmann.ac.il/~tannor> Prof. David J. Tannor, Department of Chemical Physics, Weizmann Institute, Rehovot, Israel Phone:+972-8-934-2094, Fax:+972-9-934-4123

#### **POSTDOCTORAL POSITION, HANSCOM AIR FORCE BASE**

A National Research Council Associate position is available in the COCHISE (COld CHEmical Simulation Experiment) facility 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. 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. The specific research area will involve the spectroscopy and kinetics of fast nitrogen atom collisions with oxygen molecules [fast N + O<sub>2</sub> → NO(v, high J) + O] where both the precursors and the details of the very highly rotationally excited states of NO will be investigated. Please contact Steven Miller, phone (781) 377-2807, (781) 377-8900 Fax or email: [miller@plh.af.mil](mailto:miller@plh.af.mil) for further information. U.S. citizenship is required for the above positions.

#### **POSTDOCTORAL POSITION, EMORY UNIVERSITY**

I am looking for a Postdoctoral Fellow who will work in my group at Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, Atlanta, Georgia, USA. Please send CV and publication list directly to me, preferably via e-mail. Also make arrangement to have at least two letters of recommendation (preferably from former advisers) directly to me.

The postdoctoral fellow will be involved in

Theoretical studies of potential energy surfaces of excited electronic States for photochemical and ion-molecule reactions of small gas phase molecules.

The position can start in the fall 1999, or early 2000. The appointment is originally for one year, but an extension to the second year is possible with mutual agreement.

Keiji Morokuma, William H. Emerson Professor of Chemistry, Department of Chemistry, Director, Cherry L. Emerson Center for Scientific Computation, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, USA Phone (404) 727-2180; Fax (404) 727-6586, E-mail: [morokuma@emory.edu](mailto:morokuma@emory.edu)

Web: <http://euch4m.chem.emory.edu/>

#### **POSTDOCTORAL POSITION, EMORY UNIVERSITY**

A POSTDOCTORAL POSITION at the US Naval Academy is available to study atomic-scale adhesion and tribology that occur at solid-solid interfaces in hydrocarbon- and silicon-containing systems using molecular dynamics starting October 1, 1999. Experience with computer simulations and FORTRAN is required. The position may be expanded to include the teaching of midshipmen if desired. (A second position may be available pending funding approval.) Send vitae, transcripts, and 3 letters of recommendation to Professor

Judith A. Harrison, US Naval Academy, Chemistry Department, Annapolis, MD 21402-5026. EMAIL: jah@nadn.navy.mil, VOICE: (410) 293-6624, FAX (410) 293- 2218. The Naval Academy is an Equal Opportunity employer.

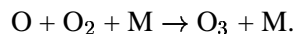
### **POSTDOCTORAL POSITION, INDIANA UNIVERSITY**

A postdoctoral position is available in my group. The position involves the use of plane wave based density functional theory to study problems in surface catalysis. However, the postdoctoral will also work on novel new variations of Vanderbilt-type pseudopotentials to reduce memory requirements of plane wave codes. Finally, the postdocoral student will be involved in a collaboration with Wavefunction Incorporated to produce a user friendly plane wave based density functional theory program suitable for use on PC's and an associated training manual for use of experimental materials scientists as well as undergraduate students studying solid states physics. A successful postdoctoral will likely be a strong candidate for a permanent position at Wavefunction, Inc.

Professor Glenn J. Martyna, Department of Chemistry, Indiana University, Bloomington, IN 47405-4001  
Phone: (812)-855-6605, Fax: (812)-855-8300, Email: martyna@martynal.chem.indiana.edu

### **POSTDOCTORAL POSITIONS, LOS ALAMOS NATIONAL LABORATORY**

It appears very likely that we will soon have openings for two postdoctoral associates. These positions will be available from October 1, 1999 onward. Both involve theoretical calculations of three-body collision processes in atomic and molecular recombination and collision-induced dissociation. Each successful candidate is expected to engage in research on one of the following two fascinating but challenging projects. One project is to explain theoretically the large, anomalous isotope effects that experimentalists have observed in the formation reaction of ozone,



These calculations will be carried out using semiclassical wavepacket propagation techniques and will involve methods development, programming, and computation. They will also involve exact quantum mechanical calculations of all the bound vibrational and rotational states of the isotopic variants of ozone using hyperspherical methods.

The other project is to calculate the rates of three-body recombination of Alkali atoms ( $A = \text{Li, Na, K, etc.}$ ),  
 $A + A + A \rightarrow A_2 + A,$

at the ultracold temperatures of Bose-Einstein condensates, using hyperspherical methods. It will also involve methods development, programming and computation.

Candidates must: 1. Have received the PhD degree in Chemistry or Physics or a closely related field within the past three years.

2. Be skilled in atomic and molecular quantum scattering theory.

3. Be a theoretician. (If you are an experimentalist, please do 4. Be expert in programming and computation using large Fortran computer codes.

5. Have a record of demonstrated research accomplishments.

In addition, the successful candidate for the first project should have had experience with classical trajectory calculations on atomic and molecular systems.

Successful candidates will work with Russell T Pack, Robert B. Walker, Brian K. Kendrick and other members of the theoretical chemistry and molecular physics group.

Outstanding candidates will have the opportunity to compete for prestigious LANL fellowships.

For consideration, please submit a resume and publications list including the names of three people who will provide references to Russell T Pack at pack@lanl.gov.

The salary depends on the length of time since the PhD; for a new PhD is is \$48,900 per year. The appointment is initially for 1 year with renewals possible up to three years. For more details about the LANL postdoctoral program see <http://www.hr.lanl.gov/html/postdoc> and the web pages linked to it.

The positions will be open to non-US citizens as well as US citizens.  
Los Alamos National Laboratory is an Affirmative Action/Equal Opportunity Employer.

### **POSTDOCTORAL POSITION, UNIVERSITY FREIBURG**

A postdoc/research associate position is available at the Institute for Theoretical Quantum Dynamics. The project is concerned with the development of time-dependent methods to describe the femtosecond dynamics and spectroscopy of nonadiabatic molecular processes. In particular, we are interested in (i) classical and semiclassical methods, (ii) time-resolved femtosecond spectroscopy, and (iii) microscopic models for photobiological processes. The position is granted for 18 months (beginning 1 Aug 1999) and is (most likely) extended for three more years. Salary is according to BAT IIa (ca. 70 000 DM/year). The position is granted for 18 months (beginning 1 Aug 1999) and is (most likely) extended for up to three more years. Applicants should send a curriculum vitae, publication list and a brief statement of research interests. PD Dr. Gerhard Stock, Faculty of Physics, University Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Telephone: +49-761-203-5956, Fax: -5883, stock@physik.uni-freiburg.de,  
<http://tqd1.physik.uni-freiburg.de/~stock>

### **POSTDOCTORAL POSITION, UNIVERSITY COLLEGE LONDON**

A Postdoctoral Research Fellowship in THEORETICAL SURFACE SCIENCE / MOLECULAR QUANTUM DYNAMICS is available in the group of Peter Saalfrank at the Chemistry Department, University College London. The position is funded by the EPSRC (Engineering and Physical Sciences Research Council).

TOPIC, GENERAL: Quantum theory of adsorbate manipulation at surfaces

TOPIC, SPECIAL: Theory of STM (Scanning Tunnelling Microscope) manipulation of atoms (e.g., H) or molecules at surfaces (e.g., Si). The "manipulation" includes the active lateral or vertical motion, or the excitation and control of internal degrees of freedom.

- Methods: Ab initio quantum chemistry; time-dependent wave packet propagation; open-system density matrix propagation using "direct" or stochastic wave packet methods.

STARTING DATE: November 1st, 1999, or October 1st, 1999.

DURATION: 12 months are guaranteed; I'm trying to get funding for longer.

SALARY: Ca. 18,900 GBP/yr + 2,134 GBP/yr London allowance

NEEDED: A PhD in theoretical physics or theoretical chemistry

WANTED: - Training or working knowledge in one or more of the following areas: ab initio quantum chemistry, numerical molecular reaction theory, wave packet propagation, density matrix propagation, numerical quantum optics.

- Good background in computation.

- Knowledge of solid state physics and / or surface science.

If interested, please send (until 15 September) a curriculum vitae, a list of publications, and a summary of research interests and skills to the address given below. I'll be pleased to answer any questions, or to give further information.

PETER SAALFRANK, University College London, Chemistry Department & Centre for Theoretical and Computational Chemistry (CTCC), Christopher Ingold Laboratories, 20 Gordon Street, London WC1H 0AJ, United Kingdom

Tel: ++44-171-504 4635, Fax: ++44-171-380 7463, Email: p.e.saalfrank@ucl.ac.uk

<http://calcium.chem.ucl.ac.uk/webstuff/people/saalfrank>

### **POSTDOCTORAL POSITION, SRI INTERNATIONAL**

The Physics and Atmospheric Chemistry (PAC) Unit of the Molecular Physics Laboratory (MPL) is searching for well-qualified candidates for a post-doctoral position in experimental physical chemistry. The

work involves collision energy transfer studies of excited states of molecular oxygen and nitric oxide, typically by means of pump-and-probe ionization techniques, under the supervision of Dr. Richard Copeland and Dr. Tom Slanger. These studies are directed towards an improved understanding of upper atmospheric processes. In recent years, the collisional energy transfer rates and pathways of all the oxygen electronic states lying below the first dissociation limit have been studied, even including the quintet state that had long been hypothesized as a possible atmospheric precursor. Nitric oxide is an important trace gas in the upper atmospheres of both the terrestrial and Venusian atmospheres, and its two metastables are to be investigated as part of a program to study auroral processes. These investigations connect to field observations, as we are learning to take advantage of the fact that large telescopes around the world routinely generate spectra of the terrestrial night airglow that are far better in terms of resolution, sensitivity, and spectral coverage than has previously been available.

SRI International is a not-for-profit contract research organization, located in Menlo Park, California, in the San Francisco Bay region, and is one of the largest such establishments in the world. Many areas of research are represented by the investigations carried out at SRI, including chemistry, physics, engineering, life sciences, computer sciences, education, and a variety of other disciplines. MPL has an international reputation for creative and innovative research in atmospheric studies, combustion processes, surface science, plasma research, and molecular beam research. Within MPL, the members of the PAC unit have been active for many years in studying the chemistry and physics of the atmosphere, with Drs. Copeland and Slanger's emphasis on the processes that occur in the 80-120 km night airglow region. There has been close coupling between the laboratory kinetics studies that this group carries out, and the results of optical emission studies by field observers.

We expect the candidate to have experience in the operation and maintenance of pulsed laser systems. Other qualifications include a Ph.D. degree in chemistry or physics, and beyond laboratory abilities, effective technical writing is an important attribute for the position, as well as an ability to make oral presentations. Appointment is typically for a minimum of one year, with a second year normally being available upon mutual agreement. The salary will depend on the experience of the candidate.

A CV, three letters of recommendation, and a one page "research interests" summary should be sent to: Dr. Richard A. Copeland, PS091, Molecular Physics Laboratory, SRI International, Menlo Park, California 94025. Telephone: (650) 859-6534

#### **POSTDOCTORAL POSITION, UNIVERSITY OF ROME**

An experimental position to work on a molecular beam apparatus for the study of Helium droplets and clusters in their interactions with electrons and with molecular 'impurities' is available in the group of Prof. F.A. Gianturco, in collaboration with Prof. A. Giardini and Dr. D. Stranges. The position is open to German candidates through the Feodor Lynen Fellowships of the Van-Humboldt Stiftung. The work is directed to the study of the dynamics and kinetics of reactive processes involving negative ions in He droplets or in small helium clusters. Interested candidates should have experience with a molecular beam apparatus, and possibly with electron guns, and should be able to interact with a supporting theory group. For further details contact F.A. Gianturco at FAGIANT@CASPUR.IT. Starting time by direct arrangement with the candidate.

#### **POSTDOCTORAL POSITION, UNIVERSITY OF ROME**

The Theoretical Chemical Physics group of Professor. F.A. Gianturco offers a Postdoctoral Position supported by the Max-Planck-Research Foundation for work on the dynamics of molecular impurities in Rg clusters (chiefly in He clusters) and on the nature of their structures, of their behaviour with electron scattering and of their interaction forces. The candidates are expected to have a working knowledge of both quantum molecular scattering theory and classical molecular dynamics. For further details contact F.A. Gianturco (FAGIANT@CASPUR.IT). Expected starting time: fall 1999.

## b. Preprints

### **Reactive scattering of oxygen and nitrogen atoms**

Acc. Chem. Res.

P. Casavecchia, N. Balucani, M. Alagia, L. Cartechini, and G.G. Volpi

Dipartimento di Chimica, Universit di Perugia, 06123 Perugia, Italy piero@dyn.unipg.it

### **Crossed beam studies of reaction dynamics**

Annu. Rev. Phys. Chem., Vol. 50

P. Casavecchia, N. Balucani, and G.G. Volpi

Dipartimento di Chimica, Universite di Perugia, 06123 Perugia, Italy piero@dyn.unipg.it

### **Exploring the reaction dynamics of nitrogen atoms: A combined crossed beam and theoretical study of $N(^2D)+D_2 \rightarrow ND+D$**

J. Chem. Phys. (Comm.) Vol. 110 (18) (8 May 1999)

M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia, and G.G. Volpi

Dipartimento di Chimica, Universite di Perugia, 06123 Perugia, Italy piero@dyn.unipg.it

L. A. Pederson and G.C. Schatz

Department of Chemistry, Northwestern University, Evanston, Illinois 60208-3113

G. Lendvay

Institute of Chemistry, Hungarian Academy of Sciences, H-1525 Budapest, P.O.B. 17, Hungary

T. Hollebeek, T.-S. Ho, and H. Rabitz

Department of Chemistry, Princeton University, Princeton, New Jersey 08544-1009

### **Crossed beam studies of the $O(^3P, ^1D)+CH_3I$ reactions: Direct evidence of intersystem crossing**

Faraday Discuss. 113 "Stereochemistry and control in Molecular Reaction Dynamics"

M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia, M. van Beek, and G.G. Volpi

Dipartimento di Chimica, Universite di Perugia, 06123 Perugia, Italy piero@dyn.unipg.it

L. Bonnet and J.C. Rayez

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

### **Shell-Like Features and charge localisation in protonated Helium clusters**

in: **Quantum Systems in Physics and Chemistry** (R. Mc Weeny and R. Wilson Eds.) 1999

I. Baccarelli, B. Balta, V. Aviyente, C. Saluki, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The effect of an helium cluster environment on the proton is studied using ab initio, correlated calculations.

### **Spatial structures and electronic excited states of small protonated helium clusters**

Int. J. Quantum Chem.

I. Baccarelli, F.A. Gianturco\*, F. Schneider

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

Excitation energies and spatial configurations are obtained for the smaller He clusters around a proton using MRD-CI methods.

### **Dynamics of ionic microsolvation: the protonated Ar clusters**

Chem. Phys. Phys. Chem.

F. Filippone, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The ab initio molecular dynamics approach is employed to study the structures and configurations for small Ar clusters enclosing a proton.

### **Intermolecular forces from density functional theory: a multiproperty analysis for Ar-CO**

J. Chem. Phys.

F. Paesani, M. Laranjeira, V. Vassilenko, M.A. da Cunha, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The VdW interaction is computed using a combination of ab initio methods and perturbation theory. The results are compared with transport coefficients.

### **Comparative configurational studies of He, Ne and Ar trimers**

J. Chem. Phys.

T. Gonzalez-Lezana, J. Robajo-Soneira, S. Miret-Artes, G. Delgado-Barrio, P. Villarreal, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The possible structures of the lower bound states of the title systems are obtained using distributed Gaussians.

### **Screening ionic motion in sodalite cages: a dynamical study**

F. Filippone, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The insertion of a screened proton using small He clusters is studied by ab initio dynamics.

### **Computed elastic cross sections and angular distribution of low energy electron scattering from gas phase fullerene.**

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

R.R. Lucchese, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The scattering of electrons from fullerene is performed for the first time using ab initio methods. Good accord is found with experiments.

### **Electron attachment to C<sub>60</sub> molecules**

Chem. Phys. Lett.

F.A. Gianturco\*, R.R. Lucchese

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The attachment of electrons to C<sub>60</sub> is studied in terms of dominant partial waves at threshold.

### **On the resonant features of electron scattering from ozone**

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

R. Curik, F.A. Gianturco, N. Sanna

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The measured resonant features for O<sub>3</sub><sup>-</sup> temporary ions are reproduced using different theoretical scattering models.

### **Protonated Ozone: structure, energetics and nonadiabatic effects**

J. Phys. Chem.

M. Ceotto, M.H. Hirst, F.A. Gianturco\*

Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy.

The possible structures of (O<sub>3</sub>H)<sup>+</sup> are computed with high accuracy and possible conical intersections are examined.

### **The dynamics of the O(<sup>1</sup>D) + N<sub>2</sub>O → NO + NO reaction revisited: a QCT study on model potential energy surfaces**

Chemical Physics Letters

Miguel Gonzalez\* (a), D. Troya (b), M.P. Puyuelo (b), R. Sayos (a), P.A. En rriquez (a)

(a) Centre de Recerca Quimica Teorica i Departament de Quimica Fisica, Universitat de Barcelona, C/ Marti i Franques, 1, 08028 Barcelona, Spain.

(b) Departamento de Quimica, Universidad de La Rioja, C/ Obispo Bustamante, 3, 26004 Logrono, Spain.

The dynamics of this reaction has been studied using the QCT method on three different triatomic LEPS PES model. On the basis of the experimental vibrational distributions and QCT results, it is suggested that the  $\text{NO}(v'=16, 17) + \text{NO}(v'=0)$  state-specific reaction channel is not majoritary. However, is about this channel that most of the reaction dynamics information is available. A quite good description of the dynamics of this specific channel has been obtained. We have also shown that for a very exoergic reaction without a strong kinematic constraint, like the one under consideration, the vector relation  $j^2 = \alpha l$ , with  $\alpha$  being a constant, can occur if the PES has no barrier or a negligible one along the minimum energy path and is highly isotropic.

### **Ab initio potential energy surface, VTST and QCT study of the $\text{O}(^3\text{P}) + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$ reaction**

Journal of Chemical Physics

Miguel Gonzalez\* (a), J. Hernando (a), J. Millan (b), R. Sayos\* (a)

(a) Centre de Recerca Quimica Teorica i Departament de Quimica Fisica, Universitat de Barcelona, C/ Marti i Franques, 1, 08028 Barcelona, Spain.

(b) Departamento de Quimica, Universidad de La Rioja, C/ Obispo Bustamante, 3, 26004 Logrono, Spain.

An ab initio study of the ground PES of this reaction has been performed using the second and fourth order Moller Plesset ab initio methods with a large basis set. From the ab initio data a triatomic analytical PES has been derived. This PES has been employed to study the kinetics and dynamics of this reaction. The ab initio points have also been used directly to calculate the VTST rate constant considering all the atoms of the system. The best VTST methods used lead to a good agreement with the experimental rate constant for 1000-2500 K, but the QCT ones are about one third the experimental ones for 1500-2500 K. The cold QCT  $\text{OH}(v=0)$  rotational distribution obtained is in good agreement with experiments, and the very small QCT  $\text{OH}(v=1)$  population obtained is consistent with the measurements. The triatomic PES model may be used in dynamics studies under conditions where the methyl group motions are not strongly coupled to the motions leading to reaction.

### **"Fundamentals in Chemical Physics"**

Franco Battaglia and Thomas F. George

(Kluwer Academic Publishers, The Netherlands, 1998)

This 326-page textbook, designed for advanced undergraduate and graduate students, addresses the topics of classical physics, quantum physics, thermodynamics, quantum chemistry, molecular spectroscopy, states of aggregation and chemical reactions.

### **"Computational Studies of New Materials"** edited by Daniel A. Jelski and Thomas F. George (World Scientific, Singapore, 1999)

This book consists of fourteen chapters authored by leading experts on topics including semiconductors (bulk and surfaces), fullerenes, polymers, fractal clusters, surface light-induced drift, optical phase conjugation and micro-mesoscopic optics.

### **Charge Transfer and Electron Pairing in Fullerenes**

Journal of Cluster Science

R. T. Fu, G. P. Zhang, X. Sun and Thomas F. George\*

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

The concept of self-trapping of a transferred electron in  $\text{C}_{60}$  is used to explain the main features of photoinduced electron transfer in a polymer- $\text{C}_{60}$  composite and electron pairing in alkali-metal doped  $\text{C}_{60}$ .

### **Appearance and Disappearance of Superfluid Vortices in a Narrow Annulus**

Physica B: Condensed Matter

C.I. Um, K.H. Chang and Thomas F. George\*

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

Introducing the radial deviation of a ring of vortices from its equilibrium position, a new form of critical angular velocities symmetrically changed by the deviation is obtained for three types of experiments in a narrow annulus.

### **Optical Origin of Efficient and Selective Trans-Cis Isomerization in Photexcited Polyenes**

Journal of Chemical Physics

G. P. Zhang, X. F. Zong and Thomas F. George\*

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

It is found that this highly-efficient isomerization is closely related to the highly-selective optical transitions, and the dipole-allowed transitions occur selectively around the dihedral angles of 60 degrees and 120 degrees, where the system is able to undergo cis or trans isomerization.

### **Dynamical Process of Exciton Combination in Polymers**

Journal of Chemical Information and Computer Sciences

E.H. Zhao, H. Jiang, X. H. Xu, X. Sun and Thomas F. George\*

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

Due to the one-dimensional characteristic, the excitation of an electron in polymers is self-trapped, and two excitons can be combined to form a biexciton. By solving the dynamic equations, the relaxation process of this combination is investigated, where it is found that the relaxation time is about 160 fs.

### **Kinetic Energy-Based Normal Mode Analysis of Electronic Processes in C<sub>60</sub>**

Fullerene Science and Technology

G.P. Zhang, X.Sun and Thomas F. George\*

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

The two most dominant Hg modes are identified which play an essential role in the dynamical properties of C<sub>60</sub>, which is consistent with the experimental results, which clarifies the previous theoretical ambiguity showing that the electron-phonon coupling constant is basically the same for different modes.

### **Quantum mechanical and quasi-classical rate constant calculations for the O(<sup>3</sup>P)+HCl→OH+Cl reaction**

Phys. Chem. Chem. Phys.

F. J. Aoiz, L. Banares, J. F. Castillo, M. Menendez and J. E. Verdasco

The dynamics of the hydrogen exchange reaction at 2.20 eV collision energy: comparison of experimental and theoretical differential cross sections

### **The low temperature rotational relaxation of N<sub>2</sub> studied with resonance enhanced multiphoton ionization**

J. Phys. Chem. A

F. J. Aoiz, T. Diez-Rojo, V. J. Herrero, B. Martinez-Haya, M. Menendez, P. Quintana, L. Ramonat, I. Tanarro and E. Verdasco

### **Electronic States of the Triply Charged Molecular Ion N<sub>2</sub><sup>3+</sup> and Laser Induced Coulomb Explosion**

Phys Rev A

A.D. Bandrauk

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

D.Musaev and K.Morokuma

Emerson Computational Center, Emory Univ, Atlanta, GA30322, USA

Potential energy curves for the low-lying doublet and quartet states of N<sub>2</sub><sup>3+</sup> have been obtained using ab-initio

methods. No stable bound states are found in the midst of many coulomb repulsive potentials. The most relevant configurations are enumerated for discussion of recent laser Coulomb explosion and imaging experiments.

### **Measuring Nuclear Wave Functions by Laser Coulomb Explosion Imaging** Phys. Rev. Lett.

A.D. Bandrauk, S. Chelkowski

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

P.B. Corkum

SIMS, National Research Council, Ottawa, Ont., K1A OR6, Canada

From exact non-Born-Oppenheimer simulations of dissociative-ionization of  $H_2^+$  in an intense ( $I > 10^{14}$  W/cm<sup>2</sup>), ultrashort ( $t < 5$ fs) laser pulse we show that it is possible to measure directly from the kinetic energy of coulomb exploded protons the probability distribution of any initial vibrational state or wavepacket. The theory of the inversion method is presented and its application to Laser Coulomb Explosion Imaging, LCEI, of time dependent wave packets is demonstrated through numerical simulations.

### **Intense Field ionization of Molecules by Ultra-Short Laser Pulses**

Comments Atom. & Molec. Phys.

A.D. Bandrauk

Labo de Chimie Theorique, Univ de Sherbrooke, Que, J1K 2R1, Canada

Exact numerical solutions of the time-dependent Schrodinger equation of one and two electron molecular ions in short ( $t < 50$ fs) intense ( $I > 10^{14}$  W/cm<sup>2</sup>) laser pulses show that molecular ionization rates exhibit unusually large values at critical configurations, interfragment distances  $R_c$  and internal angles  $\phi_{ic}$ . Large charge resonance radiative couplings are shown to be responsible for the large ionization rates called Charge Resonance ionization, CREI. Exact non-Born-Oppenheimer calculations on molecular dissociative ionization of  $H_2^+$  confirm the role of CREI as a "universal" phenomenon in recent Coulomb Explosion experiments.

### **Crossed beam reaction of the cyanogen radical, $CN(X^2\Sigma^+)$ , with methyl acetylene, $CH_3CCH(X^1A_1)$ : Observation of cyanopropyne, $CH_3CCCN(X^1A_1)$ , and cyanoallene, $H_2CCCHCN(X^1A')$**

J. Chem. Phys. (submitted)

L.C.L. Huang, Y. Osamura, N. Balucani, Y.T. Lee, R.I. Kaiser

Institute of Atomic and Molecular Sciences, Taiwan, ROC

### **A versatile source to produce high intensity, pulsed supersonic radical beams for crossed beam experiments - the cyanogen radical, $CN(X^2\Sigma^+)$ , as a case study**

Rev. Sci. Instr. (submitted)

R.I. Kaiser, J. Ting, L.C.L. Huang, Y.T. Lee, H. Chan, D. Stranges, D. Gee

Institute of Atomic and Molecular Sciences, Taiwan, ROC

### **Ionic Fragmentation of Methyl Methacrylate Induced by Synchrotron Radiation and Multiphoton Ionization**

Journal of the Brazilian Chemical Society, v.9, n.6, (1998) 521-24.

Cristina M. Quintella, G. Gerson B. de Souza and Joselito B. Maciel

Inst. Quimica, Univ. Fed. Bahia, Brasil / Inst. Quimica, Univ. Fed. Rio de Janeiro, Brasil

Ionic fragmentation of MMA has been observed using either Laser MPI (2.35eV) or Synchrotron PI (from 12.1eV to 287.9eV), coupled to a time-of-flight technique. The fragmentation pattern remains the same in both PI cases. MPI causes extensive fragmentation, the parent ion can not be observed and  $C^+$  becomes the most intense fragment. Very stable ions are observed at  $m/q = 15, 39, 41$  and  $69$ .

### **New Way of Controlling Molecular Processes by Time-Dependent External Fields**

J. Chem. Phys.

Yoshiaki Teranishi and Hiroki Nakamura\*

Dept. Theor. Studies, Inst. Molec. Science, Myodaiji, Okazaki 444-8585, Japan

Molecular processes in external fields are considered to be composed of a sequence of time-dependent nonadiabatic transitions in which the external fields play a role of adiabatic parameters. Unit final transition probability can be achieved by sweeping the field periodically at each avoided crossing. The idea is quite general and various control schemes can be proposed. The methods of pi-pulse and chirped laser pulse with the adiabatic rapid passage may be considered as special cases of the present idea.

### **Molecular Switching in a Two-Dimensional Constriction**

J. Chem. Phys.

Hiroki Nakamura

Dept. Theor. Studies, Inst. for Molec. Science, Myodaiji, Okazaki 444-8585, Japan

The new idea of molecular switching discussed previously for the one-dimensional system is extended to a two-dimensional constriction model. Both reflection and transmission, and thus the switching cannot be complete like in the one-dimensional case, but the switching is demonstrated to be quite effective. Some practical implications are discussed.

## **c. Conferences**

### **1. ACCADEMIA NAZIONALE DEI LINCEI**

Perugia, Italy, Dipartimento di Chimica dell' Universite, 19 June, 1999

Centro Interdisciplinare "Beniamino Segre" Giornata Lincea "Molecular Aspects of Gas Dynamics"

Perugia, Italy: Dipartimento di Chimica dell' Universite

Scientific Committee: V. Aquilanti, S. Carra', C. Cercignani, G.G. Volpi

9.00 - Welcome Address - Gian Gualberto Volpi (Perugia) Introduction - Sergio Carra' (Milano)

9.30 - Chair - Vincenzo Aquilanti (Perugia)

D.R. Herschbach (Harvard, Premio Nobel), Bringing molecules to attention.

R.N. Zare (Stanford, California), Reaction dynamics: the H+ D<sub>2</sub> - HD + H exchange revisited.

A. Wodtke (Santa Barbara, California), Rapid evaporative cooling suppresses fragmentation in mass spectrometry: synthesis of "Unprotonated" water cluster ions.

D. J. Nesbitt (Boulder, Colorado, Jila), Collisional Dynamics of Rotational Alignment

R. W. Anderson (Santa Cruz, California), Achromatic Lenses for Molecules.

15.00 - Chair- Sergio Carra' (Milano)

J.K. Harvey (Imperial College, London), The application of Direct Simulation Monte Carlo techniques to plasma problems

Jean-Claude Lengrand (CNRS Meudon, Paris), Rarefaction Regimes and Thermodynamic Nonequilibrium

Mario Capitelli (Bari), From plasmas to hypersonic and nozzle flows

Aldo Frezzotti (Milano), DSMC Simulation of Dense Gases

Conclusions - Carlo Cercignani (Milano),

For information: bellini@dyn.unipg.it Dr. David Cappelletti, Fax: (39) 75 585 5606, e-mail:

prometeo@dyn.unipg.it, URL: <http://www.chm.unipg.it/chimgen/mb/mb.html>

### **2. MOLECULAR REACTION DYNAMICS**

University of Birmingham, 8 JULY 1999

The Second Meeting of the University of Birmingham Centre for Chemical Physics to be held in the School of Chemistry at The University of Birmingham on Thursday 8th July 1999. This meeting is being held in conjunction with the Northern Universities' Meeting on Chemical Physics

The University of Birmingham has established a cross-disciplinary Centre for Chemical Physics. It formalises and extends existing links between research groups in the Schools of Chemistry and Physics bringing together researchers with a wide range of interests in chemical physics including: the dynamics of neutral-neutral and ion-molecule reactions, the physics and chemistry of the gas-solid interface, the chemistry and physics of free and adsorbed clusters, electronic structure and scattering calculations, laboratory astrophysical chemistry, and the use of vacuum ultraviolet radiation, including femtosecond sources to probe the dynamics of gas-phase and surface species.

This meeting features a number of invited speakers:

DJ Auerbach (IBM San Jose)

DJ Nesbitt (JILA, University of Colorado, Boulder)

GC Schatz (Northwestern University)

AG Suits (Lawrence Berkeley National Laboratory)

The Centre for Chemical Physics gratefully acknowledges generous sponsorship from Nicolet Instruments Ltd in support of this meeting and its seminar programme.

### **3. GORDON CONFERENCE DYNAMICS OF SIMPLE SYSTEMS IN CHEMISTRY AND PHYSICS**

Salve Regina University in Newport, RI, 11-16 July, 1999

The 1999 Gordon Research Conference "Dynamics of Simple Systems in Chemistry and Physics" will be held 11-16 July at Salve Regina University in Newport, RI.

The program focuses on few-body problems in atomic, molecular, chemical, and nuclear physics. Details can be found at the website

<http://tangelo.phys.unm.edu/~chandler/gc.html>

Financial assistance is available (through the generosity of the National Science Foundation and the Office of Naval Research), especially for graduate students and junior post doctoral scientists.

Applications for financial assistance should be directed to the Chair (Colston Chandler, [chandler@unm.edu](mailto:chandler@unm.edu)).

Questions about all other matters should be directed to the Chair or to the Vice Chair (Paul Julienne, [paul.julienne@nist.gov](mailto:paul.julienne@nist.gov)).

### **4. GORDON CONFERENCE IN QUANTUM CONTROL OF ATOMIC AND MOLECULAR MOTION**

Plymouth State College, Plymouth, NH, August 1-6

Contributed talks will be given in the following areas: Wavepacket Dynamics, Coherent Phase Control, Wave Properties of Matter, Optimal Control, Quantum Computing, Control in Condensed Phases, Intense Field Control, N-Level Systems, Decoherence and Dephasing

Invited speakers and session chairs include: Andre Bandrauk, Chris Bardeen, Klass Bergmann, Phil Bucksbaum, Dimitris Charalambidis, Paul Corkum, David Cory, Louis diMauro, Dan Elliott, Gustav Gerber, Martin Gruebele, Stephen Harris, Lene Hau, Albert Heberle, Bob Jones, Paul Julienne, Ronnie Kosloff, Jeff Krause, Oleg Prezhdo, David Pritchard, Herschel Rabitz, Mark Raizen, Stuart Rice, Marlan Scully, Moshe Shapiro, Yaron Silberberg, John Sipe, David Tannor, David Wineland, Yijin Yan, and Wojciech Zurek.

The conference chairs are Paul Brumer and Robert Gordon. A complete schedule of the sessions and a list of the lecture titles are found at the website:

<http://www.grc.uri.edu/programs/1999/quantcon.htm>

The conference will include several poster sessions, and participants in the conference are urged to present their latest results.

A limited amount of funds are available to defray part of the costs of attending the conference. Applications for support should be sent to either of the chairs at [pbrumer@tikva.chem.utoronto.ca](mailto:pbrumer@tikva.chem.utoronto.ca); or [rjgordon@uic.edu](mailto:rjgordon@uic.edu) before May 15

Robert J. Gordon, Department of Chemistry (m/c 111), University of Illinois at Chicago, 845 West Taylor Street, Chicago, IL 60607-7061  
Phone: (312) 996-3280, Fax: (312) 996-0431, email: rjgordon@uic.edu

## **5. GORDON CONFERENCE DYNAMICS AT SURFACES**

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

Chair: Aart Kleyn, FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, kleyn@amolf.nl

Vice-Chair: Bruce Kay, Pacific NW Natl Lab, Environm Mol Sci Lab, Richland, WA, bruce.kay@pnl.gov

All general information concerning the Gordon Conferences can be found at the GRC-web-site:

<http://www.grc.uri.edu/>. Information concerning the conference is posted at the Gordon Conference site.

Conference program:

Interactions with prepared molecules:

Discussion leader: Greg Sitz (Univ. Texas at Austin)

Arthur Utz (Tufts University): Eigenstate-resolved measurements of methane dissociation on Ni(100)

Alec Wodtke (UCSB) & Daniel Auerbach (IBM Almaden): Control of reagent vibration: a key to understanding chemical dynamics at surfaces?

Dynamics at Ice:

Discussion leader: Greg Kimmel (Pacific Northwest):

Andrew Graham (MPI Goettingen): Dynamics at the ice surface observed with helium atom scattering:

Hannes Jonson (Washington): Theoretical calculations of diffusion and island formation on ice Ih surfaces.:

Jim Cowin (Pacific Northwest): Soft-landed hydronium studies of ion transport and hydration:

Excitation and charge Transfer:

Discussion leader: John Tully (Yale)

Bill Gadzuk (NIST): Breathing mode excitation in near-harmonic systems.

Barbara Cooper (Cornell): Dynamics of multi-state charge transfer.

Nano-Tribology and clusters:

Discussion leader: J. Frenken (Leiden)

Jacqueline Krim (North Carolina State): Nano tribology.

Bo Persson (FZ Julich): Atomic scale friction.

John Weaver (Minnesota): The formation of nanoclusters and their interaction with surfaces.

Vibrational spectroscopy:

Discussion leader: Akio Yoshimori (Okayama)

Maki Kawai (RIKEN): Molecule-substrate and inter-molecular interactions on metal surfaces.

Wilson Ho (Cornell): Single molecule vibrational spectroscopy and chemistry

Photo-Dynamics and Chemistry:

Discussion leader: Ian Harrison (Virginia)

Dinko Chakarov (Chalmers): Photoinduced processes at the graphite/ice interface

Ronnie Kosloff (JILA & Hebrew University): Theory of surface photochemistry

Ulrich Hfer (MPQ Garching): Wave packet dynamics of image states.

Quantum level interactions:

Discussion leader: Stephen Holloway (Liverpool)

Geert-Jan Kroes (Leiden): Quantum dynamics of H<sub>2</sub>-surface interactions.

Stig Andersson (Chalmers): Dynamics of adsorbed H<sub>2</sub>.

Surface Reactions:

Discussion leader: Gill Nathanson (Wisconsin)

Buddie Mullins (Univ. Texas at Austin): Precursors in activated dissociative chemisorption.

Tim Minton (Montana State): Reactive scattering dynamics of fast atoms with surfaces

Fleming Besenbacher (Aarhus): Nanocatalysis studied by STM

Best young researcher contributions: Discussion leader: Bruce Kay (Pacific Northwest)

Conference chair:

Prof. Dr Aart W. Kleyn, Leader, Molecular Beams Group, FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands Phone (31)-20-6081310 (direct), (31)-20-6081234 (reception), (31)-20-6279191 (home)

Fax (31)-20-6684106 (reception), (31)-20-6081288 (secretary), Email KLEYN@AMOLF.NL

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

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

## **7. 25th International Symposium on Free Radicals**

Flagstaff, Arizona, August 15-20, 1999.

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

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

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

### **SCIENTIFIC PROGRAM**

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

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

## **8. ELECTRONICALLY NONADIABATIC PROCESSES IN GASEOUS, CLUSTER AND CONDENSED MEDIA**

ACS National Meeting in New Orleans, Louisiana, August 22-26, 1999.

We are writing to encourage you to contribute to the international symposium entitled "Electronically Nonadiabatic Processes in Gaseous, Cluster and Condensed Media" at the ACS National Meeting in New Orleans, Louisiana, August 22-26, 1999.

The symposium includes the elucidation of electronically nonadiabatic effects using experiment and electronic structure theory and quantum reaction dynamics theory. We include a wide range of reactive processes in gaseous and condensed media including photochemistry, ion chemistry, physical organic mechanisms, cluster dynamics, and photosynthesis. The symposium will last four days (seven half day sessions plus one joint half day with another Symposium entitled "Imaging in Chemical Dynamics") and is the largest sponsored by the Physical Chemistry Division at this ACS Meeting. Its goal is to bring together experimentalists and theorists who are active in gas- and condensed- phase reaction dynamics, in order to present state-of-the-art measurements and calculations to encourage cross-fertilization between the researchers in different fields.

Laurie Butler, Dept. of Chemistry, Univ. of Chicago, 5640 S. Ellis Ave., Chicago, IL 60637, (773) 702-7206, fax (773) 702-5863, ljb4@midway.uchicago.edu

Don Truhlar, Dept. of Chemistry, Univ. of Minnesota, Minneapolis, MN 55455, (612) 624-7555, fax (612) 626-9390, e-mail: truhlar@umn.edu

Invited Speakers include:

Millard Alexander, University of Maryland; Dr. Mutsumi Aoyagi, Institute for Molecular Science, JAPAN; V. Ara Apkarian, University of California, Irvine; Gabriel G. Balint-Kurti, University of Bristol; Paul F. Barbara, University of Texas, Austin; Bill Breckenridge, University of Utah; Robert J. Buenker, Bergische Universitaet; David F. Coker, Boston University; Karl F. Freed, University of Chicago; Michael D. Hack, University of Minnesota; Martin Head-Gordon, University of California, Berkeley; Michael F. Herman, Tulane University; Paul L. Houston, Cornell University; Brian Kendrick, Los Alamos National Laboratory; Karl L. Kompa, Max-Planck Institut fuer Quantenoptik; Horst Koeppel, Universitaet Heidelberg, GERMANY; Marsha I. Lester, University of Pennsylvania; Raphy Levine, The Hebrew University of Jerusalem; Carl Lineberger, JILA, University of Colorado; Todd J. Martinez, University of Illinois, Urbana; Bill Miller, University of California, Berkeley; Hiroki Nakamura, Institute for Molecular Science; David Nesbitt, JILA, University of Colorado; Daniel Neumark, University of California, Berkeley; Simon W. North, Texas A&M University; Robert Parson, JILA, University of Colorado; John Polanyi, University of Toronto; Michael A. Robb, King's College London; George C. Schatz, Northwestern University; Reinhard Schinke, Max-Planck Institut, Goettingen; Benoit Soep, CNRS, Universite Paris Sud; Gerhard Stock, University of Freiburg; Peter J. Wagner, Michigan State University; Hans-Joachim Werner, University of Stuttgart; David Yarkony, Johns Hopkins University;

## 9. IMAGING IN CHEMICAL DYNAMICS

ACS National Meeting in New Orleans, Louisiana, August 22-26, 1999.

We are organizing a symposium entitled "Imaging in Chemical Dynamics" at the 218th national meeting of the American Chemical Society in New Orleans, LA from August 22-26, 1999. Imaging methods have had a profound impact on the study of chemical dynamics in recent years, and the field is now in a state of explosive growth in applications and methodology. Applications of imaging techniques to photodissociation, inelastic and reactive scattering, photoionization and photodetachment processes will be among the topics addressed by the invited speakers. It is hoped that this symposium will serve to document 'state-of-the-art' imaging applications in chemical dynamics, showcasing the growth in the field and the range of the experimental possibilities. In this announcement, we would like to encourage submission of contributed talks and posters to highlight some of the newest results in this symposium. We hope to put together a book documenting the current state of the field in the ACS symposium series and look forward to your contribution.

Invited speakers include:

Musahid Ahmed, LBL (Berkeley); John Barker, Michigan State; Richard Bersohn, Columbia; David W. Chandler, Sandia (Livermore); Robert Gordon, University of Illinois, Chicago; Carl Hayden, Sandia (Livermore); Paul Houston, Cornell; Bill Jackson, UC Davis; Dennis Jacobs, Notre Dame; A. Khai Luong, UC San Diego; Theo Kitsopoulos, University of Crete / IESL-FORTH; Kopin Liu, IAMS (Taipei); George McBane, Ohio State; Dan Neumark, UC Berkeley; David Parker, Nijmegen; Andrei Sanov, Univ. of Arizona; Toshinori Suzuki, IMS (Okazaki); Wim Van der Zande, FOM (Amsterdam); Oleg Vasyutinskii, Ioffe-St Petersburg

The symposium will include a joint half-day session with the Symposium on "Electronically Nonadiabatic Processes in Gaseous, Cluster and Condensed Media" organized by Laurie Butler and Don Truhlar.

Organizers:

Robert E. Continetti, Dept. of Chemistry and Biochemistry, 0314 University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0314. Tel: 619-534-5559, FAX: 619-534-7244, e-mail:

rcontinetti@ucsd.edu

Arthur G. Suits, MS 6-2100, Chemical Sciences Division, Lawrence Berkeley National Lab, Berkeley CA 94720. Tel: 510-486-4754, FAX: 510-486-5311, e-mail: agsuits@lbl.gov

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

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

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

**11. CCP5 ANNUAL MEETING 1999**

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

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

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

Invited speakers:

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

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

Dr. John Harding, Department of Physics & Astronomy, University College London, E-mail [j.harding@ucl.ac.uk](mailto:j.harding@ucl.ac.uk)

Dr. David Heyes, Department of Chemistry, School of Physical Sciences, University of Surrey, E-mail [d.heyes@surrey.ac.uk](mailto:d.heyes@surrey.ac.uk)

Dr. Maurice Leslie, CLRC Daresbury Laboratory, Daresbury, E-mail [m.leslie@dl.ac.uk](mailto:m.leslie@dl.ac.uk)

Conference timetable:

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

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

Oxford, 13 and 14 September 1999

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

### **13. ChemInt'99**

The ChemInt'99 draft program is now available at the conference web site: [www.chemint.org](http://www.chemint.org). The list of all invited speakers and virtually all panel members is now complete and listed in the program. ChemInt'99 will be held in at Georgetown University in Washington DC on September 25-27, 1999. Poster talks/papers submissions will be accepted only via the web site starting in the spring.

The main lecturers for the meeting will be:

Alan Arnold, University College (UNSW); Steven Bachrach, Northern Illinois University; Robert Bovenschulte, ACS; Stephen Boyer, IBM; Karl Harrison, Oxford University; Clemens Jochum, Deutsche Bank; Gary Mallard, NIST; Tom Pierce, Rohm & Haas; Jerome Reichman, Vanderbilt; Achim Zielesny, Bayer AG; Steven S. Zumdahl, University of Illinois at Urbana-Champaign

The corporate sponsors for the meeting are: ChemWeb and the Internet Journal of Chemistry

ChemInt web site <http://www.chemint.org>

### **14. HIGHLY EXCITED ELECTRONIC STATES**

Sant Feliu de Guixols, Spain, 23-28 October 1999

On behalf of Dr Tim Softley (Oxford) and Professor Klaus Mueller-Dethlefs (York), we are proud to announce that the preliminary programme of the above-mentioned European Research Conference is now ready.

This conference aims to bring together researchers active in the field of spectroscopic and dynamical studies of highly excited electronic states of molecules (e.g., Rydberg, ion-pair or dipole bound states), including those who study the properties directly and those that make use of them in areas such as ZEKE spectroscopy, ionic state selection, Rydberg tagging etc.

If you want to have further information on the meeting (programme, list of invited speakers, availability of grants...) and to apply, please consult our web site at the following address:

<http://www.esf.org/euresco/PC99137A.HTM>

### **15. SYMPOSIUM IN MEMORY OF GERHARD HERZBERG**

Cornwall, Canada, Oct. 30- Nov. 3, 1999

Inspired by Herzberg: Spectroscopy for the Year 2000

The symposium will feature 32 outstanding invited speakers, with the following topics:

- Ions and Radicals
- Rydberg States
- Astrophysics
- van der Waals Molecules
- Metal Compounds
- Theory and Techniques of Spectroscopy

For more information, check out our web site:

[www.sims.nrc.ca/sims/sims\\_e.html](http://www.sims.nrc.ca/sims/sims_e.html)

or contact us at: [spectroscopy.conf@nrc.ca](mailto:spectroscopy.conf@nrc.ca)

### **16. WORKSHOP ON PHOTODYNAMICS FROM ISOLATED MOLECULES TO CONDENSED PHASES**

HAVANA, CUBA, FEBRUARY 13-19, 2000

Local Organizing Committee: Jesus Rubayo Soneira (Chairman), Juan de Dios Garrido Arrate, Mario Piris Silvera, Jesus Sabin del Valle, German Rojas Lorenzo

International Advisory Board: Majed Chergui (Switzerland), Vincenzo Aquilanti (Italy), Gerardo Delgado-Barrio (Spain), Antonio Varandas (Portugal), Julian Echave (Argentina), Jesus Rubayo Soneira (Cuba),

Invited speakers (confirmed participation) will include: Alberto Beswick (Universite Paul-Sabatier, France); Benoit Soep (Universite Paris-Sud, France); L. Woste (Freie Universitat Berlin, Germany); Abdelkrim Chemseddine (Hahn - Meitner - Institut Berlin GmbH, Germany); Vincenzo Aquilanti (Universita di Perugia, Italy); Antonio Varandas (Universidade de Coimbra, Portugal); Gerardo Delgado-Barrio (CSIC, Spain); Pablo Villarreal (CSIC, Spain); Salvador Miret-Artes (CSIC, Spain); Angel Gonzalez Urenha (Universidad Complutense de Madrid, Spain); Abderrazzak Douhal (Universidad de Castilla-La Mancha, Spain); Majed Chergui (Universite de Lausanne, Switzerland); David C. Clary (University College London, U.K.); V.S. Letokhov (Academy of Science, Russia); G. Billing (University of Copenhagen, Denmark); Kenneth Janda (University of California at Irvine, U.S.A.); D. Julius Jellinek (Argonne National Laboratory, U.S.A.); A. C. Albrecht (Cornell University, U.S.A.); Donald L. Thompson (Oklahoma State University, U.S.A.); Julian Echave (Univ. Nacional de Quilmes, Argentina); Marco Antonio Chaer (UFRJ, Brazil); Sylvio Canuto (USP, Brazil); Adalberto Fazzio (USP, Brazil); Oscar Ventura (Montevideo, Uruguay); Ramon Hernandez-Lamonedada (UAEM, Mexico); Luis Javier Alvarez (UNAM, Mexico); Luis A. Montero Cabrera (Universidad de La Habana, Cuba); Jesus Rubayo Soneira (ISCTN, Cuba);

Participation: Scientists and students working or interested in the field, from both Latin- American and industrialized countries are welcome to attend. The workshop will be conducted in English. Please type, print in ink, or send by e-mail the participation form to our university.

Scope and Format The central theme of the Workshop is the description, both from the experimental and a theoretical point of view of the physical and chemical processes in molecular systems. The main topics to be covered are:

\* Dynamics and reactivity of isolated molecules.

Dynamics of molecular species embedded in small and large clusters.

Molecular dynamics of molecules in the condensed phase (liquid, solid) and at surfaces.

The scientific programme will include invited lectures, oral presentations of contributed papers and poster sessions, with ample time for discussion.

The workshop will be held in Havana, Cuba. Havana, after several settlements was finally founded in 1519 at its present location. The city came to be a highly relevant place, first of all, due to its geographic position since it is washed by the Gulf Stream and this was a determining factor for navigation at that time which depended mainly on the oceanic currents. There are important touristic and recreative resorts. The climate is wonderful ( it never snows), the mean temperature in February is 21 C.

Registration and accommodation fee. Approximately US\$ 250 before November 30-1999, US\$ 300 afterwards. The package will cover conference fees, coffee breaks, Book of Abstracts, Book of Proceedings, welcoming reception and workshop dinner. Room prices for the whole meeting, including breakfast (6 nights) will start from approximately US\$ 240 (single room) and US\$ 360 (double room). Cheaper accommodation can be arranged upon special request. More details on lodging and other activities will be given in the second announcement. Reduced price for participants from Latin-American and East-European countries will probably be available (details in second announcement).

Deadlines Mail the enclosed pre-registration form to the Organizing committee before July 15, 1999. Please feel free to use copies of the form for your colleagues as necessary. The second announcement (including registration form, call for abstracts, etc.) will be mail to those who have pre-registered. The deadline for registration and submission of abstracts will be September 1st, 1999. The final announcement (programme, travel information, etc.) will be mailed in December 1999.

For further information please contact: Jesus Rubayo Soneira, Instituto Superior de Ciencias y Tecnologia Nucleares, Ave. Salvador Allende y Luaces. Quinta de los Molinos, Habana 10600, A.P. 6163. Ciudad Habana, Cuba.

E-Mail: jrs@rsrch.isctn.edu.cu, jrs@ff.oc.uh.edu.cu, Telefax: (53-7) 785018, (53-7) 241188, Telephone: (53-7) 575662/63

Pre-registration form

NAME AND PROFESSIONAL TITLE

ADDRESS

Phone

Fax

E-mail

Please send me further information ( )

I plan to attend the workshop ( )

I intend to present a communication ( )

I request a:

Single room ( ) Double room ( )

DATE SIGNATURE

### **17. FARADAY DISCUSSION 115 MOLECULAR PHOTOIONISATION**

The University of York, 3-5 April 2000

The Faraday Discussion page (York): <http://rempi.york.ac.uk/rsconf.html>

The Faraday Discussion page: <http://www.rsc.org/lap/confs/fadmeet.htm>

Molecular photoionisation dynamics presents a challenge both from experiment and theory. New insight has come from (i) the invention of ZEKE photoelectron spectroscopy as a very high resolution tool and (ii) theoretical approaches to quantitatively understand the ionisation dynamics. There is an interest in advancing this burgeoning field and very actively studied applications come from van der Waals and hydrogen bonded molecular clusters including intra-cluster reactions, molecular Rydberg states including their time-resolved dynamics and their stability in fields, Multichannel Quantum Defect and scattering theory, Rydberg state tagging, molecular and cluster anion photodetachment, charge transfer, radicals, and correlated two-electron ionisation processes.

The discussion is intended to bring together practitioners of the broadest range of photoionisation, photodetachment and charge transfer experiments, spectroscopists, molecular physicists and theoreticians working on angular momentum transfer, scattering theory, electron correlation and non-Born-Oppenheimer effects in Rydberg states, with a view to establishing state-of-the-art applications in chemistry and molecular physics as we move into the new millennium, while focussing on the immediate future prospects of this whole area of research.

The introductory Keynote Lecture will be given by Professor B V McKoy (Pasadena).

Experimental and theoretical papers will be particularly welcome in all the areas mentioned above.

Organising Committee:

Professor K Mueller-Dethlefs (Chair), Professor M Ashfold, Professor M S Child FRS, Professor R J Donovan, Professor J M Dyke, Professor F Read FRS, Dr T P Softley

View also: The original ZEKE Home page: <http://rempi.york.ac.uk/>

and information about the ERC Highly Excited States

The ERC Conference page (York): <http://rempi.york.ac.uk/esfconf.html>

The ERC Conference page (note capitalization): <http://www.esf.org/euresco/PC99137A.HTM>

### **18. MOLECULAR and IONIC CLUSTERS CONFERENCE - 2000)**

Toulouse, France, April 16-21 2000

This conference follows a series of very successful Gordon conferences, with the last two held at Il Ciocco, Italy (1996) and Ventura, California (1998). The conferences have taken place biannually, alternating between the US and Europe. This alternation underlines the international aspect of the field and provides a regular channel for exchange between scientists in North America and Europe. The year 2000 conference will not be a Gordon conference, since the Gordon Research Conferences do not have an official site in

France. However, it will adhere to the Gordon Conference format, and be followed by a GRC planned for 2002 back in Ventura. There will be room for 120-130 participants.

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

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

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

PISA, Italy, June 12-16, 2000

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

The Conference is jointly organised by:

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

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

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

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

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Alessandro Lami, Istituto di Chimica Quantistica ed Energetica Molecolare del CNR, via Risorgimento 35, I-56126 Pisa (Italy)

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

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

## **20. MOLEC XIII (MOLEC 2000)**

Jerusalem, Israel, September 17 - 22, 2000

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

Local Organizing Committee:

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

For more information contact M. Baer at Soreq Nuclear Research Center, Yavne 81800, Israel. email:  
mmbaer@netvision.net.il  
Information also appears on the web ([www.fh.huji.ac.il/~roib/MOLEC/index.htm](http://www.fh.huji.ac.il/~roib/MOLEC/index.htm))

# Special announcement

## INVITATION TO SUBMIT A PAPER

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

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

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

Further information from:

Professor J N L Connor,

Department of Chemistry,

University of Manchester,

Manchester M13 9PL, England.

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

## BOOKS

### **Theory and Application of Quantum Molecular Dynamics**

John Z.H. Zang, published by World Scientific

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

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

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

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