

Molecular Dynamics News

numbers 103; October 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 has been accepted - otherwise state *unpublished*).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 104 to Prof. R.W. Anderson (**You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU**). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#103). The closing date for issue number 104 is December 1, 1999.

*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**

Name: _____

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GOOD NEWS FOR THE FIELD: NOBEL TO ZEWAIL

The Nobel Committee has announced that the Nobel Prize in Chemistry 1999 is being awarded to Professor Ahmed H. Zewail of Caltech. for his studies of the transition states of chemical reactions using femtosecond spectroscopy.

The full citation is available at: <http://www.nobel.se/announcement-99/chemistry99.html>

On behalf of the MDN Community, we congratulate with Ahmed.

ELECTRONIC DELIVERY OF MDN

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

1. Electronic mail to subscribers

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

2. World Wide Web

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

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

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

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

The list was created by Jeremy Hutson in June 1993 and has now more than 1600 members.

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

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

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

If you would like a list of the current members, send a message containing the line

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review molecular-dynamics-news
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to the address mailbase@mailbase.ac.uk

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

a. Open Positions

FACULTY

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.

Theoretical/Computational Chemistry Position at Emory University, Department of Chemistry

A new position in theoretical/computational chemistry at the tenure-track Assistant Professor level (under exceptional circumstances possibly at a higher level) will be available beginning the fall semester of 2000. We are interested in individuals who have a strong background in theoretical chemistry and who have interests in applications to problems at the interface between biology and chemistry. Strong commitment to teaching at graduate and undergraduate level is essential. This position is one of several that will be made in the next few years in the areas of biological and materials chemistry, as part of expansion of the department into a new 40,000 square foot facility. The theoretical position will be affiliated with the Cherry L. Emerson Center for Scientific Computation, which will move to the new building in the Fall 2000. Applicants should send a curriculum vitae, a research proposal and a short statement on teaching interest, and make arrangement to have three letters of recommendation sent directly to: Theoretical/Computational Search Committee, Department of Chemistry, Emory University, Atlanta, GA 30322. Review of applications begins on October 15, 1999, and will continue until the position is filled. Emory University is An Equal Opportunity and Affirmative Action Employer.

Department Heads for Experimental Research, Max-Planck-Institut für Strömungsforschung, Göttingen, Germany

The Max-Planck-Institut für Strömungsforschung, Göttingen, Germany, plans to expand its activity in the field of Physical Biology. The Institute seeks candidates for two Department Heads for Experimental Research (Directors at the Institute)

For further details visit our home page <http://www.mpisf.mpg.de>

The advertisement has also been published in DIE ZEIT, July 29 1999, in Nature, August 5 1999, and in Science, August 13 1999.

Three professor positions, Université de Montreal

The Université de Montreal wishes to hire three professors, one in theoretical chemistry, one in polymer/materials science, and one in analytical chemistry. All interested candidates are invited to send (by the 15th of November 1999) a CV, a research proposal, a list of equipment needs and to have letters of recommendation sent to:

The Chairman Department of Chemistry Université de Montreal Case postale 6128 succursale Centre-ville — Montreal (Quebec) H3C 3J7 — Canada

The working language of the university is French. New professors who do not already speak French must acquire an adequate knowledge of the language within a reasonable period after appointment. For more

information about the department consult the web page

POST DOCTORAL AND VISITING

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 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 Na₂ 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 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 **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, 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, 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

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

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 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

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. Argonne National Laboratory is an Equal Opportunity Affirmative Action Employer.

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 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,

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_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

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

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).

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 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 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

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

<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 weel1@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 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 $N + O_2 \rightarrow NO(v, \text{high } J) + O$] 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 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

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@nadm.navy.mil, VOICE: (410) 293-6624, FAX (410) 293- 2218. The Naval Academy is an Equal Opportunity employer.

POSTDOCTORAL POSITION, INDIANA UNIVERSITY

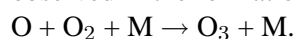
A postdoctoral position is available in my group. The position involves the use of plane wave based density functional theory to study problems in surface catalysis. However, the postdoctoral will also work on novel new variations of Vanderbilt-type pseudopotentials to reduce memory requirements of plane 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@martyna1.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 ($A = \text{Li}, \text{Na}, \text{K}, \text{etc.}$),
 $A + A + A \rightarrow A_2 + A,$

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 month (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 month (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 OAJ, 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 Slinger'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.

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>

POST-DOCTORAL POSITION AT SRI INTERNATIONAL COLLISIONAL ENERGY TRANSFER IN SMALL ATMOSPHERIC MOLECULES

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 Slinger. 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 Slinger'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 resum, 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 Illinois

It is anticipated that a postdoctoral position will become available next year in the research group of Robert Gordon at the University of Illinois at Chicago. Experiments in the areas of atomic, molecular, and chemical physics include the following:

1. Coherent control of the reactions of molecules by exploiting the interference between different excitation paths. We have already shown that one- and three-photon excitation can be used to control the branching between photoionization and photodissociation of HI and DI. Moreover, the phase lag between the two reactive channels provides a new spectroscopic tool for understanding interactions in the continuum. We wish next to extend these ideas to more complex molecules.
2. Ultrafast studies of the dynamics of pendular states. The fundamental of a Ti:Sapphire laser will be used to align a molecule, and a harmonic of this laser will be used to probe its time evolution. Experiments are also planned to study the focusing and deflection of neutral molecules.
3. Photofragment imaging of aromatic compounds. A newly constructed velocity mapping imaging apparatus is being used to study internal conversion and intersystem crossing in molecules such as iodobenzene.

Further details are available upon request. Experience with pulsed dye lasers and/or ultrafast lasers, as well as with molecular beams, is desirable. The salary range is 25,000 to 30,000, depending on experience. Interested candidates should send their resumes and the names and addresses of at least two references to: 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

Postdoctoral position, Bar-Ilan University

A postdoctoral position has become available in my group at Bar-Ilan University. The research will concern development and application of new semiclassical approximations for the dynamics and time-independent properties of atomic and molecular systems. Among general topics of interest are:

- (a) Development of new, computationally simple, integral expressions for semiclassical wave functions and propagators.
- (b) Extension of current initial value semiclassical treatments to systems that are naturally described in terms of non-Cartesian coordinates.
- (c) Efficient semiclassical treatments of scattering and spectral amplitudes.
- (d) Semiclassical calculation of atomic and molecular electronic wave functions.
- (e) Practical semiclassical treatments of deep tunneling.

The techniques developed will be applied to a variety of specific systems of chemical and physical interest. The position is available immediately but it may be possible to delay its start for a few months. The initial appointment is for one year and may be renewed upon mutual agreement. Candidates should have good mathematical backgrounds and, preferably, have experience in semiclassical theory and/or molecular reaction dynamics. To apply, send me a CV (e-mail is fine) and arrange to have three letters of recommendation sent to the address below:

Kenneth G. Kay Department of Chemistry Bar-Ilan University Ramat-Gan, Israel 52900

E-mail: kay@mail.biu.ac.il Phone: +972-3-5318722 Fax: +972-3-5351250

Research Associate / Postdoctoral Fellow in Physical Chemistry, Department of Chemistry, University of Adelaide, Australia

Gas Phase Molecular Reaction Dynamics (Ref: 3938) Salary: A\$37,779 - \$46,013*

(* a minimum rate of \$42,864 per annum is payable to the holder of a Ph.D.)

A postdoctoral position in the area of gas phase molecular reaction dynamics is available in the laboratory of Dr Mark A. Buntine. The emphasis of the project is on the elucidation of the structure and reactivity of microsolvated negative ion clusters. Current target systems include hydrated anions such as superoxide, O_2^- ,

and hypochlorite, OCl^- . The experiments utilise a tandem time-of-flight mass spectrometer incorporating a pulsed cluster source. One- and two-colour laser-based anion photodetachment and photodissociation studies form the basis of the project. The successful candidate will be expected to develop novel two-colour stimulated Raman methodologies to complement the existing spectroscopic techniques. The experiments are supported by ab initio computational studies of ion cluster geometries and potential energy surfaces as an aid to interpretation of the experimental results.

This contract position is available immediately for a period of 12 months in the first instance with the possibility of an extension into a second year.

Applicants should possess:

A Ph.D. in chemistry, physical chemistry, or chemical physics or have submitted their Ph.D. thesis.

Demonstrated experience with high vacuum systems and pulsed, tunable laser systems.

Excellent written and oral communication, laboratory and computing skills.

An awareness of recent chemistry literature relevant to gas phase physical chemistry, including familiarity with automated chemical literature searching databases.

An awareness of laboratory safety and occupational health issues and equal opportunity policies.

Experience with pulsed optical parametric oscillator (OPO) systems, and ab initio computational chemistry methods would be an advantage.

Interested applicants should contact Dr Mark A. Buntine via email, fax, or mail for further information, including the selection criteria.

Formal applications, including Curriculum Vitae and certified academic transcripts should be directed to the address below. Applicants should also arrange to have three letters of recommendation sent directly to the address below: Dr Mark A. Buntine, Department of Chemistry, The University of Adelaide, Adelaide, SA 5005; Phone: +61-8-8303-5580; Fax: +61-8-8303-4358; email: mark.buntine@adelaide.edu.au
Applications close 31 October, 1999.

Postdoc position, University of Florida

A postdoc position is available at the NSF-KDI center, University of Florida. The responsibility associated with this position is to develop and implement DFT method and DFT based molecular dynamics to study chemical-mechanical processes such as chemical reaction dynamics at tip of cracks in materials, chemical reaction dynamics at surface in chemical-mechanical polishing process, and stress corrosion in metals. The focus of this position is electronic structure and dynamics at surfaces using both finite cluster model and band structure calculation approach, using classical as well as DFT based first principle simulations. The overall project of KDI center is on multi-scale simulation of materials behavior including chemical reactivities. The goal is to develop a theoretical framework that integrate quantum-chemistry/DFT/semi-empirical-approaches/classical-MD to study material properties and processes at various spatial and temporal scale.

Requests for further information and applications should be addressed to:

Prof. Hai-Ping Cheng and/or Prof. Sam Trickey Department of Physics & QTP University of Florida Gainesville, FL 32611 Phone: (352)-392-1597 Fax: (352)-392-8722 email: cheng@qtp.ufl.edu and/or trickey@qtp.ufl.edu URL <http://www.qtp.ufl.edu>

POST DOCTORAL RESEARCH ASSISTANTSHIP IN LASER PHOTOCHEMISTRY, School of Chemistry, UNIVERSITY OF BRISTOL

Applications are invited for a 30 month Post Doctoral Research Assistantship, funded by the Leverhulme Trust in the group of Professor M N R Ashfold from 1.1.2000 or as soon thereafter as is mutually convenient. The work will involve substantial extensions of the existing H atom photofragment translational spectroscopy experiment so as to allow:

(i) quantitative high resolution studies of the primary photochemistry of a range of prototypical hydrides at

user selected wavelengths in the vacuum ultraviolet,

(ii) investigation of the photochemistry (and thermochemistry) of ≈ 20 jet-cooled free radical hydrides and
(iii) exploration of the vibrationally mediated photodissociation of hydride molecules.

For recent illustrations of work under this program see *Journal of Chemical Physics*, 110, 281 (1999)
Phys.Chem.Chem.Phys., 1, 45 (1999); 1, 767 (1999); 1, 3247 (1999). and
<http://www.chm.bris.ac.uk/laser/laserhom.htm>.

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 \approx £317,238 - \approx £319,869 per annum according to age and experience. Informal enquiries can be addressed to mike.ashfold@bris.ac.uk.

Applications, which should include a CV and the names of two referees, must be sent to the Personnel Office (University of Bristol, Senate House, Bristol BS8 1TH, Tel: 0117 954 6947, minicom 0117 928 8894 or email: Recruitment@bris.ac.uk) quoting reference 5841 by the closing date: 15 November 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
<http://www.bris.ac.uk/Depts/Chemistry/staff/aoewing.htm>

POST-DOC Position(s) at Max-Planck-Institut fuer Chemie, Mainz, Germany

I am looking for a post-doc to come and work in Mainz on a pulsed laser photolysis (PLP) experiment with pulsed laser induced fluorescence (PLIF) and resonance fluorescence (RF) detection of radicals and atoms. Investigations of atmospheric kinetics and photochemical processes that influence the HO_x and NO_x families are planned. The position could start in January or sooner if desired.

In addition, position(s) will be available from January onwards to investigate heterogeneous reactions taking place on/in atmospherically relevant surfaces/solutions (e.g. ice, H₂SO₄, sea-salt) using laminar flow tube/mass spectrometer methods.

In both cases salaries would be based on an "Auslandsstipendium" (foreign scholarship) which is 3600 DM (tax-free) per month. For German nationals other arrangements would be available. Experience with lasers is highly desirable for the PLP-PLIF experiments. The positions could initially be for 2 years, with the possibility of extension.

Further information about the group and current activities is found at my web site.

John Crowley

Postdoctoral position in theoretical chemistry, University of California

A postdoctoral position is available in the group of Prof. Craig C. Martens at the University of California, Irvine. Opportunities exist for contribution to two general research areas:

–The development and application of semiclassical methodology for modeling dynamics and ultrafast spectroscopy in many-body systems. This project focuses on treating ultrafast photodynamics, nonadiabatic dynamics, electronic dephasing, many-body tunneling, and other physical problems using methods based on the semiclassical limit of the quantum Liouville equation.

–Studies of many-body ultrafast dynamical phenomenology and theoretical spectroscopy in far-from-equilibrium systems using molecular dynamics simulation and analytic methods. This project combines large-scale molecular dynamics simulation of the nonlinear many-body dynamics of condensed phase systems with the development of new analytic approaches to describing these challenging problems and the design of new experimental (or gedanken-experimental) techniques that allow the resulting novel ultrafast phenomena to be observed and characterized.

(Reprints and preprints containing more information are available upon request.)

The successful applicant will have a strong background and interest in one or more of the following areas: large-scale molecular dynamics simulation methodology, theoretical aspects of nonlinear spectroscopy,

nonadiabatic molecular dynamics, nonlinear dynamics, semiclassical mechanics.

Please send an application, consisting of a curriculum vitae, brief statement of research interests and experience, and two or more letters of recommendation, to:

Craig C. Martens Department of Chemistry University of California, Irvine Irvine, CA 92697-2025
cmartens@uci.edu

Complete application by email is acceptable (and encouraged).

Short Post-Doctoral Appointment in Ab Initio Calculation of Combustion Dynamics in the research group of Prof. G.G. Balint-Kurti (University of Bristol, U.K.)

A short appointment of about 4.5 months is available immediately in the research group of Professor G.G. Balint-Kurti (University of Bristol, U.K.) to study combustion dynamics processes using ab-initio quantum mechanical methods. The work will involve large scale ab initio electronic structure calculations of reaction paths and rate constant calculations using our own RRKM codes.

Applications should be accompanied by a CV and the names and addresses of two referees. They may be sent by email to: Gabriel.Balint-Kurti@bristol.ac.uk or by post to:

Professor G.G. Balint-Kurti School of Chemistry University of Bristol Bristol BS6 6LY U.K.

PS It may be possible to extend the duration of the appointment to a maximum of 7.5 months depending on the permission of the granting agency and the date of uptake of the appointment.

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

Postdoctoral Position in Theoretical Chemistry, University College London

A postdoctoral position is available in the group of Professor David Clary to develop new quantum mechanical methods to calculate the vibrational states of weakly-bound molecular trimers. The position is available from January 2000 and will last for up to three years. It is funded by the EPSRC.

University College London is one of Europe's leading universities and is a major centre for Theoretical and Computational Chemistry. It is situated in the heart of one of the world's most exciting cities. The Clary group is lively and international, and the computational facilities are excellent.

Theoretical chemists or physicists who are interested in this position should email David Clary (d.c.clary@ucl.ac.uk) in the first instance. Full applications will require a curriculum vitae and the names of two referees. The closing date for applications is October 1 1999.

More information on the group and UCL can be obtained from the web site

<http://calcium.chem.ucl.ac.uk/webstuff/people/clary/pubs/index.html>

Professor David C Clary, FRS Centre for Theoretical & Computational Chemistry Department of Chemistry University College London 20 Gordon Street London, WC1H 0AJ, UK

Postdoctoral or visiting scholar position, Chemistry Divison, Argonne National Laboratory

A postdoctoral or visiting scholar position is available in the Chemistry Divison of the Argonne National Laboratory in the area of theoretical and computational studies of atomic clusters. The studies cover a broad variety of physico-chemical properties of clusters (structural and dynamical) and of cluster-related phenomena, including cluster-molecule and cluster-substrate interactions. Both, homogeneous and heterogeneous, e.g., alloy, systems are considered. The work involves analytical and methodological developments, code development, and large-scale computer simulations. Excellent computational resources are available. Candidates with background in quantum chemistry, theoretical chemistry and/or solid state physics, classical and quantum dynamics, and related fields are wellcome to apply. The appointment is initially for one year with a possible extension upon mutual agreement. Interested candidates should forward their CV and list of publications and arrange for three recommendation letters to be sent to Dr. Julius Jellinek Chemistry Division Argonne National Laboratory Argonne, Illinois 60439 USA E-mail: JELLINEK@ANLCHM.CHM.ANL.GOV Tel.: (630)252-4729 FAX: (630)252-4954

Postdoctoral position, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan

A postdoctoral position is available in my group in the Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan. The work involves applications of accurate quantum chemical ab initio methods (CCSD(T), MRCI, CASSCF, CASPT2, modern DFT, etc.) to the studies of electronic and vibronic spectra of various molecules and radicals through calculations of excited electronic states, potential energy surfaces for chemical reactions, and photodissociation dynamics, related to combustion, atmospheric and interstellar chemistry. The position is available immediately. The appointment is originally for one year, but an extension is possible with mutual agreement. Please send CV and publication list directly to me, preferably via e-mail. Also make arrangement to have two letters of recommendation directly to me.

Alexander M. Mebel Assistant Research Fellow Institute of Atomic and Molecular Sciences Academia Sinica P.O. Box 23-166, Taipei, Taiwan 10764 Tel.: (886)-2-2366-8208 Fax : (886)-2-2362-0200 e-mail: mebel@po.iams.sinica.edu.tw

POSTDOCTORAL FELLOWSHIP IN ATMOSPHERIC CHEMISTRY SCHOOL OF CHEMISTRY, UNIVERSITY OF LEEDS

A postdoctoral position is available immediately at Leeds in the atmospheric chemistry group. The project will involve field work (with some instrument development) and/or numerical modelling, related to the measurement of OH and HO₂ radicals in the troposphere by laser-induced fluorescence (using the FAGE instrument). The appointment is for one year in the first instance, with an extension subject to mutual agreement and funding.

The salary will be on the scale for Research Staff Grade IA according to qualifications and relevant experience.

Please contact Dr. Dwayne Heard, tel. + 44 (0) 113 233 6471; fax +44 (0) 113 233 6565; email dwayneh@chem.leeds.ac.uk for further details about the project. Information regarding the research activities of the atmospheric chemistry group and about the School of Chemistry can be found at: <http://www.chem.leeds.ac.uk>

Applicants should send as soon as possible (by email, fax or mail) a detailed CV together with the names, phone numbers and e-mail addresses of two referees to: Dr. D. E. Heard, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK.

The University of Leeds promotes an Equal Opportunities Policy.

Dr. Dwayne E. Heard, School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK. Tel: 0113 2336471 Fax: 0113 2336565 dwayneh@chem.leeds.ac.uk <http://chem.leeds.ac.uk/Atmospheric/Field/field.html> <http://www.chem.leeds.ac.uk/People/Heard.html>

**Postdoctoral Research Associate in Theoretical Molecular Physics
Department of Physics and Astronomy, UNIVERSITY COLLEGE LONDON**

An EPSRC funded Postdoctoral Research Assistantship in Theoretical Molecular Physics is available for a period of up to 30 months. The post is to work with Prof Jonathan Tennyson and Dr Lesley Morgan on low-energy electron-molecule collisions using the R-matrix method. The project would suit a candidate with a background in either atomic and molecular physics or quantum chemistry. The appointment would be on the lower part of the Research Staff Scale 1A, currently £16,286 – £23,521 p.a. plus £2134 London weighting.

Further information can be obtained from: Jonathan Tennyson, Department of Physics & Astronomy, University College London, Gower Street, London WC1E 6BT, UK Tel: +(44) 171 380 7809 Fax: +(44) 171 380 7145 Email: j.tennyson@ucl.ac.uk

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

Applicants should send a curriculum vitae, including the names of two referees, as soon as possible to Prof

Jonathan Tennyson.

Postdoctoral Position, Institute of Atomic and Molecular Sciences (IAMS), Chemical Dynamics Laboratory, Taiwan

Two postdoctoral positions are available immediately in the research group of Dr. Kopin Liu at IAMS, Taiwan. The current experimental programs include (i) developing a novel scheme of coherent control of molecular photodissociation, and (ii) crossed-beam studies of radical reaction dynamics. Both projects are fairly challenging and involve various state-of-art experimental techniques. Additional information can be found at <http://kliu.iams.sinica.edu.tw/>. Experience with molecular beam and/or laser spectroscopy is strongly preferred, however, the most critical criterion is creativity. The initial appointment will be for one year, with the expectation of renewal for a second year contingent upon reasonable progress. The starting monthly salary is about US\$2,000, and one-way airfare to Taiwan will be reimbursed.

Applications with two letters of recommendation, a curriculum vitae and a list of publications should be sent to:

Dr. Kopin Liu, Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei 10764, Taiwan Fax: 886-2-2362-0200 email: kpliu@gate.sinica.edu.tw <http://kliu.iams.sinica.edu.tw/>
Kopin Liu IAMS, Academia Sinica, P.O.BOX 23-166 Taipei, Taiwan 10764
FAX:886-2-23620200 TEL:886-2-23668259
<mailto:kpliu@gate.sinica.edu.tw> <http://kliu.iams.sinica.edu.tw/>

University of Utah, Chemistry Department Computer Professional

Network administrator having experience managing Sun Solaris 2.5, 2.5 and 7, Linux, Irix, MacIntosh, and Windows 95/98/NT. Additionally, this person must be able to manage the Microsoft SQL server (version 7) software and must be proficient with Microsoft Access.

Network experience: Experience with switched, routed and repeated networks. Experience with Cabletron and Cisco routers is necessary for management of the firewall and the modem pool. Must be well versed with TCP/IP and its related protocols/services including DNS and SMTP. Experience with Sendmail, Postfix, TCP wrappers, SATAN and Crack is required. Experience with firewalls is necessary to maintain network security. Experience with DNS is required for management of IP numbers and their associated names (i.e. chemistry.chem.utah.edu).

Experience with twisted-pair ethernet, thinwire ethernet, fast ethernet and gigabit ethernet is also required. Experience with Sun Net Manager is a plus.

A background in chemistry is very useful, as it helps identify computer and network needs for the various groups.

Experience with networks serving 300-400 users and 300-400 machines is a must.

This person must be able to handle multiple jobs at once and prioritize them appropriately.

Experience with electrical systems and air conditioning systems is a plus.

Salary \$45-46K per year plus benefits.

Send applications to:

Human Resources, 1901 East South Campus Drive, Salt Lake City, UT 84112.

You can print the application off the web at: <http://www.personnel.utah.edu/forms/afe.pdf>

Gregory A. Voth, Ph.D. Professor of Chemistry and Director of the Henry Eyring Center for Theoretical Chemistry

Department of Chemistry and Henry Eyring Center for Theoretical Chemistry University of Utah 315 S. 1400 E. RM Dock Salt Lake City, Utah 84112-0850

(801) 581-7272 (office) (801) 581-4353 (fax) (801) 581-5419 (secretary) Email:

voth@chemistry.chem.utah.edu Web Site: <http://voth.hec.utah.edu/>

Postdoctoral Research Associate in Experimental Positron Physics, Department of Physics and Astronomy, UNIVERSITY COLLEGE LONDON

An EPSRC funded Postdoctoral Research Assistantship in Experimental Positron Physics is available for a period of up to 24 months. The post is to work with Dr Gaetana Laricchia on positron and positronium collisions with atoms and molecules. The project would suit a candidate with a background in experimental positron physics and/or atomic and molecular physics. The appointment would be on the lower part of the Research Staff Scale 1A, currently £16,286 £23,521 p.a. plus £2134 London weighting.

Further information can be obtained from: Dr Gaetana Laricchia Department of Physics and Astronomy University College London Gower Street London WC1E 6BT, UK

g.laricchia@ucl.ac.uk <http://phys.ucl.ac.uk/~ajg/> <http://www.tampa.phys.ucl.ac.uk/new/amp/>

phone: 44-(0)20-7679 3470 (direct line) 44-(0)20-7679 3485 (secretary) fax 44-(0)20-7679 2564 or 44-(0)20-7679 7145

Applicants should send a curriculum vitae including the names of two referees as soon as possible to Dr Gaetana Laricchia.

Post Doctoral Position, Tropospheric Particulate Measurements, University of Waterloo

The position will be available early in 2000. The research in our group involves the development and application of spectroscopic methods for the measurement of the physical and chemical properties of tropospheric aerosols, with emphasis on urban particulates. The candidate would be involved in the development of laser spectroscopic measurements for the chemical speciation of urban particulates. In addition to laser-based techniques, we also use FTIR for particulate characterization, and we hope to add mass spectrometry in the near future. The candidate would have the opportunity to initiate projects using these other methods as well.

The laboratory participates in a wide variety of collaborations with industry as well as Federal and Provincial governmental air quality authorities. Part of the work would involve field campaigns organized and/or funded by these agencies. We have recently undertaken a regional tropospheric modelling project and we expect that the characterization techniques developed in the laboratory will be used in the development of computational models of urban aerosol chemistry.

Preference will be given to candidates having experience with laser spectroscopic methods. Familiarity with atmospheric chemistry and analytical methods is an advantage. General information about all current projects in our laboratory may be obtained at our website: www.science.uwaterloo.ca/~sloanj.

The University of Waterloo, which has more than 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. Additional information about the University is available from <http://www.UWaterloo.CA/>.

The position is for one year initially, with the option for extensions, subject to mutual agreement and the availability of funds. Applicants should forward a CV and two letters of reference to:

Prof. J.J. Sloan Department of Chemistry University of Waterloo Tel: 1 519 888 4401 Waterloo ON N2L 3G1 Fax: 1 519 746 0435 Canada. e-mail: sloanj@UWaterloo.CA

Postdoctoral Position, Department of Chemistry, Wayne State University, Detroit

Postdoctoral Position with Dr. Evelyn Goldfield

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 the 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 development of reduced dimensionality approximate methods for studying 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>.

An Institute for Scientific Computing has recently been formed at WSU, fostering interdisciplinary interaction among researchers in a broad range of disciplines from the sciences, social sciences, engineering and medicine.

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 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.

b. Preprints

Microscopic Theory of Thin Liquid Helium Films in the Ring-Diagram Approximation

Progress in Low Temperature Physics

Chung-In Um, Lakshmi N. Pandey, Thomas F. George*

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

A review of experiments and a microscopic theory of two-dimensional superfluid helium derived in the ring-diagram approximation is presented. At very low temperatures and long wavelengths, the anomalous excitation spectrum obtained in this approximation exerts strong influences on the interactions between elementary excitations. Through the effects of three-phonon processes, the superfluid density, thermodynamics, phonon decay, various sounds and kinetic coefficients are analyzed and compared with experiments.

UV Laser-Induced Liquid-Phase Palladium Seeding on Polymers

Journal of Materials Research

K.Kordas, J. Bekesi, K. Bali, R. Vajtai, L. Nanai, S. Leppavuori and Thomas F. George*

Excimer laser pulses with wavelength of 308 nm, repetition rates of 1-10 Hz, pulse energies of 300-400 mJ and pulse width of 20 ns are used to selectively seed palladium aggregates from a liquid-phase solution on polymer (polyimide) surfaces. The palladium deposits appear as amorphous and Pd[111] crystallites forms depending on the number of laser pulses, and the roughness of a PI surface prior to seeding is modified mechanically and characterized by its fractal dimension.

High-order Symplectic Integration: an Assessment

Ch. Schlier and A. Seiter

Fakultaet fuer Physik, Hermann-Herderstr.3, D-79104 Freiburg

As a sequel to our earlier paper (JPC A, 102, 9399, 1998) we tested three new symplectic integrators of order 8, and show their advantage for accurate calculations of long classical trajectories.

The reaction of O(¹D) with H₂O, D₂O monomers and clusters and the intracomplex reaction in N₂O-X₂O (X=H,D) photo-initiated at 193 and 212.8 nm

J. Chem. Phys.

K. Imura, M. Veneziani, T. Kasai, and R. Naaman*

Department of Chemical Physics, Weizmann Institute, Rehovot, Israel

Analytical Treatment of Singular Equations in Dissociative Recombination

Comp. Phys. Comm.

Lukas Pichl, Hiroki Nakamura and Jiri Horacek

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

The Lippman-Schwinger type singular integral equation, which arises in the multi-channel quantum defect theory of dissociative recombination process, is investigated. The singularity of its kernel is treated analytically by introducing an energy dependent quadrature. In many cases of physical interest the energy-dependent coupling potential, which gives the integral kernel of the equation, is quasi-separable in a way that allows to write down an analytical solution. The analytical treatment as well as the new solution are illustrated by taking the H_2^+ as an example. Our method is demonstrated to be much better than the conventional ones, such as the first order perturbation theory and the grid method.

On the J-Shift Approximation in Quantum Reaction Dynamics

J. Phys. Chem.

Katsuyuki Nobusada and Hiroki Nakamura

Dept. Theor. Stud., Inst. Molec. Sci., Myodaiji, Okazaki 444-8585, Japan

The validity of the J-shift or energy-shift approximation is investigated numerically by taking the reaction $\text{O}(^3\text{P})+\text{HCl} \rightarrow \text{OH}+\text{Cl}$ as an example. The approximation based only on the results of J (total angular momentum quantum number)=0, which is the ordinary J -shift approximation, cannot reproduce the exact reaction dynamics well, especially when the initial rotational quantum number is high. The reaction rate constants for specified initial rovibrational states are over- or underestimated depending on the initial state and temperature. The good agreement with the accurate result of the thermal rate constant seems to be rather accidental because of the cancellation of these over- and underestimates. An extended J -shift approximation is proposed, in which accurate calculations should be carried out up to $J = j_i$ with $|\Omega| \leq \Omega_{max}$ when $j_i \leq \Omega_{max}$, or up to $J = \Omega_{max}$ when $j_i > \Omega_{max}$, where Ω_{max} is the maximum of the absolute values of the body-fixed projection quantum number Ω that give noticeable contributions to the reaction dynamics. When the maximum J required to have a well converged cross-section and rate constant is much larger than j_i , it is recommended to carry out accurate calculations at some representative J values and to use these values to estimate probabilities at other J values by an appropriate interpolation or extrapolation procedure.

Ab initio ground potential energy surface and QCT study of the $\text{O}(^1\text{D}) + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$ reaction dynamics

Journal of Chemical Physics

Miguel Gonzalez *, Jordi Hernando, Irene Banos, and R. Sayos *

Departament de Química Física, Universitat de Barcelona C/ Martí i Franques, 1. 08028 Barcelona, Spain

$\text{O}(^1\text{D})+\text{CH}_4$ reaction, ground potential energy surface, ab initio calculations, triatomic analytical fitting, quasiclassical trajectory calculations.

Statistics of energy levels in the quantum treatment of an elementary reaction

Gaia Grossi, Leonardo Peroncelli

Dipartimento di Chimica dell'Università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy

Naseem Rahman

Dipartimento di Scienze Chimiche dell'Università di Trieste

Via Giorgieri 1, 34127 Trieste, Italy

Statistical tests (NNLSD, Δ_3 of Dyson and Mehta, correlation coefficients) are applied to the adiabatic energy level distribution of the prototypical reaction $\text{F} + \text{H}_2 \rightarrow \text{HF} + \text{H}$, depending parametrically on the three-body total inertia

measured by the hyperradius ρ . As a function of ρ (proposed as a natural control variable for the quantum mechanical three-body problem), a transition can be identified. At high ρ the situation of separate partners of the reaction shows a Poissonian behavior, while at low ρ the transition state (where the triatom can be viewed as a system of coupled oscillators) exhibits some Wigner-like features as signatures of quantum chaos.

Molecular beam scattering of aligned oxygen molecules. The nature of the bond in the O₂-O₂ dimer

Journal of American Chemical Society, in press (1999).

V.Aquilanti, D.Ascenzi, M.Bartolomei, D.Cappelletti, S.Cavalli, M.de Castro Vitores, and F.Pirani

Molecular beam experiments are reported for collisions between oxygen molecules. Total integral cross sections have been measured as a function of the collision energy and with the control of molecular alignment. This first complete experimental characterization of the interaction yields a ground (singlet) state bond energy of 17.0 ± 0.8 meV for the most stable dimer geometry at a distance of 3.56 ± 0.07 Å. Also the splittings among the singlet, the triplet and the quintet surfaces are obtained and a full representation of their angular dependence is reported via a novel harmonic expansion functional form for diatom-diatom interactions.

Chemiluminescent reactions of excited calcium atoms with HCl and HBr: selective charge-transfer "harpooning" and synchronized intermediate complex rearrangement

J. Phys. Chem.

M. De Castro, R. Candori, F. Pirani, V. Aquilanti

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

Macarena Garay, Angel González Ureña

Unidad de Laseres y Haces Moleculares, Instituto Pluridisciplinar, Universidad Complutense de Madrid, 28040 Madrid, Spain

A "harpooning" mechanism is investigated for the chemiluminescent reactions of Ca* (¹D₂) atoms with HCl (leading to CaCl* in the A state) and with HBr (leading to CaBr* in both the A and B states). A model of the interactions in the entrance channels, which involves an electron jump and leads to a charge-transfer intermediate complex, accounts for the selective dependence of reactivity on the relative orientation between the molecule and the outer electronic orbital of the atom. The dynamical treatment incorporates in the Landau-Zener approach the synchronization between times for nonadiabatic transitions and for triggering the rearrangement of the intermediate collision complex. The treatment accounts for the observed features of the translational energy dependence of the cross-sections: the steep initial increase with a pronounced maximum, the sharp decline and also fine details, such as a stair-like behavior.

c. Conferences

1. 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>

2. 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

or contact us at: spectroscopy.conf@nrc.ca

3. 1999 Waterloo Symposium on Chemical Physics

Waterloo, Ontario, will be held on the weekend of November 5-7

The fifteenth annual Symposium on Chemical Physics at the University of Waterloo in Waterloo, Ontario, will be held on the weekend of November 5-7, 1999. As usual, the Symposium will include both invited and contributed oral papers, as well as a Poster session, and will run from approximately 7:30 PM on the Friday evening till mid-day Sunday. The Saturday afternoon Poster session and reception will be followed by the conference banquet and the usual extended discussions. The Invited Speakers for this year's meeting are:

Paul Corkum (NRC, Ottawa; Plenary Lecturer), "Strong Fields Molecular Optics"

Kelly Chance (Harvard-Smithsonian Observatory), "Fitting Atmospheric Spectra in the Infrared Through Ultraviolet: Exercises in Spectroscopy and Radiative Transfer"

James Farrar (Rochester), "Electronic Spectroscopy of Mass-Selected Clusters: Probes of Ion Solvation"

Wolfgang Jaeger (Alberta), "Spectra of van der Waals Complexes: Fingerprints of Intermolecular Interactions"

David Pratt (Pittsburgh), "Static and Dynamic Properties of Molecular Assemblies in the Gas Phase"

Jonathan Tennyson (London), "Assigning the Spectrum of Water on the Sun and Elsewhere"

Following the regular meeting, a Post-Conference Workshop on "Fitting of Atmospheric Spectra: Detailed Examples of the Process" led by Kelly Chance (Harvard-Smithsonian Astrophysical Observatory) will be offered on the afternoon of Sunday November 7. Further information is available on the conference WWW site.

FULL DETAILS regarding registration, contributed paper submission, housing and other matters, together with programs of previous meetings in this series may be found on our WWW site:

<http://theochem.uwaterloo.ca/watscp.html>

Waterloo is located approximately one hour (60 miles) from the Toronto International Airport. For further information, please contact any member of the local organizing committee.

Local Organizing Committee:

=====

P.F. Bernath, (519)888-4567, ext. 4814 (bernath@UWaterloo.ca) J.W. Hepburn, (519)888-4567, ext. 4065 (hepburn@UWaterloo.ca) R.J. Le Roy (519)888-4567, ext. 4051 (leroy@UWaterloo.ca) F.R. McCourt (519)888-4567, ext. 3024 (mccourt@UWaterloo.ca) T.B. McMahon, (519)888-4567, ext. 4591 (mcmahon@UWaterloo.ca) J.J. Sloan, (519)888-4567, ext. 4401 (sloanj@UWaterloo.ca)

4. SASP 2000 - Symposium On Atomic and Surface Physics and related topics

Hotel Biancaneve, Folgaria (Trento) Italy,

January 30 - February 5, 2000

Chair: Davide Bassi and Paolo Tosi

The XII edition of the Symposium of Atomic and Surface Physics and related topics will be held in Folgaria (Trento) Italy from January 30 to January, 2000. As usual, SASP 2000 will have a format similar to that of a Gordon Conference, with about 20 hours of lectures, 10 hours of poster presentations and ample time for discussions.

Deadlines:

Registration: July 30, 1999; Payment of the conference fee: October 28, 1999; Submission of papers for proceedings: November 15, 1999

The Preliminary List of Review Lecturers includes:

S. Cavalli (Perugia, Italy); F. De Martini (Roma, Italy); G. Gerber (Wuerzburg, Germany); F. Huisken (Goettingen, Germany); Cheuk-Yiu NG (Iowa, USA); S. Price (London, UK); J.P. Schermann (Villetanuese, France); S. Schlemmer (Chemnitz, Germany).

In addition, about 15 invited progress reports will be presented on various topics.

Poster presentations are welcome on the following topics:

Quantum optics, Atomic and molecular spectroscopy, Elementary processes in the gas phase, Structure and dynamics of clusters, Surface Physics, Applications of ion processes (astrophysics, plasmas, environment,...)

5. Seventh Laser Applications to Chemical Analysis Meeting

Santa Fe, New Mexico, February 11-14, 2000

I would like to advertise the Seventh Laser Applications to Chemical Analysis Meeting that will be held in Santa Fe, New Mexico, February 11-14, 2000. The abstracts are electronically submitted and are due September 22, 1999. The details are available on the web at: http://www.osa.org/mtg_conf/2000/lacea/

This topical meeting of the Optical Society provides a forum to discuss new spectroscopic techniques, instrumentation, and optical sources and their application to chemical analysis and environmental monitoring.

The invited presentations include:

Diode laser-based tunable UV sources for combustion diagnostics, by Daniel Oh, Southwest Sciences

A fast chemical sensor for environmental trace gas flux, by Peter Werle, Fraunhofer Institute for atmospheric Environmental Research, Germany

Kinetics of single DNA unwinding by rep helicase, Taekjip Ha, Stanford University

Bioanalytical applications of single molecule detection, R. A. Keller, Los Alamos National Laboratory

Microfabricated fluidic devices: new approaches to chemical measurements, J. M. Ramsey, Oak Ridge National Laboratory

Micro-optical systems for laser-induced fluorescence in capillary separations, by M. Warren, Sandia National Laboratory

Multidimensional fluorescence spectroscopy of single molecules, by C. Seidel, Max Planck Institute, Germany

Diode and optically-pumped mid-IR lasers based on antimonide type II W quantum wells, J. Meyer, Naval Research Laboratory

The Program Committee:

David Rakestraw, Sandia, co-chair Alan Stanton, Southwest Sciences, co-chair Markus Sauer, Heidelberg, co-chair Mark Allen, PSI Robert Shaw, Oak Ridge Volker Sick, Michigan William Ambrose, Los Alamos Doug Baer, Stanford Jay Jeffries, SRI Kevin McNesby, ARL Peter Werle, Fraunhofer Institute

This meeting has a long history of excellent contributed oral and poster presentations. I hope you will consider attending.

Jay B. Jeffries Molecular Physics Laboratory SRI International 333 Ravenswood Ave. Menlo Park, CA 94025

voice 650-859-6341 fax 650-859-6196 Jeffries@crvax.SRI.com

6. WORKSHOP ON PHOTODYNAMICS FROM ISOLATED MOLECULES TO CONDENSED PHASES (SEE ALSO THE SPECIAL ANNOUNCEMENT FOR CONTRIBUTED PAPERS!)

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); Juergen A.W. Brickmann (Darmstadt University of Technology, Germany); Vincenzo Aquilanti (Università di Perugia, Italy); Anna Giardini (Università "La Sapienza", Roma, 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 Complutence de Madrid, Spain); Abderrazzak Douhal (Universidad de Castilla-La Mancha, Spain); Florentino Borondo (Universidad Autónoma de Madrid, Spain); Majed Chergui (Universite de Lausanne, Switzerland); David C. Clary (University College London, U.K.); Frank Wilkinson (Loughborough University, U.K.); G. Billing (University of Copenhagen, Demmark); Kenneth Janda (University of California at Irvine, U.S.A.); D. Julius Jellinek (Argone National Laboratory, U.S.A.); A. C. Albrecht (Cornell University, U.S.A.); Steve Berry (University of Chicago, U.S.A.); Donald L. Thompson (Oklahoma State University, U.S.A.); Roger E. Miller (University of North Carolina, U.S.A.); J. Kerry Thomas (U.S.A.); Edwin Quiñones (Universidad de Puerto Rico, Puerto Rico); Juan Lopez Garriga (Universidad de Puerto Rico, Puerto Rico); Julian Echave (Univ. Nacional de Quilmes, Argentina); Jorge Mahecha Gomez (Universidad de Antioquia, Colombia); Marco Antonio Chaer (UFRJ, Brazil); Sylvio Canuto (USP, Brazil); Adalberto Fazzio (USP, Brazil); Ramon Hernandez-Lamoneda (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 December 15, 1999. Please feel free to use copies of the form for your colleagues as necessary. The deadline for submission of abstracts will be December 15, 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

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

For transfers and hotel reservations, please establish contact with:

Travel Agency (Agencia de Viajes) San Cristobal S.A.

Oficios no. 110 (bajos) e/. Lamparilla y Amargura

CO10100, Habana Viaja, Ciudad de La Habana, Cuba

Telephone: (53-7) 33 9585

Telefax: (53-7) 33 9586

E - mail: reservas@sancrist.get.cma.net

7. 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>

8. MOLECULAR and IONIC CLUSTERS CONFERENCE - 2000

Toulouse, France, April 16-21 2000

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

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

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

Philippe BRECHIGNAC

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Fax: +33 (0)5 61 55 60 65

Here is the address for the web site: <http://irsamc1.ups-tlse.fr/irsamc/mic2000.htm>

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

PISA, Italy, June 12-16, 2000

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

The Conference is jointly organised by:

- Istituto di Chimica Quantistica ed Energetica Molecolare del CNR, Pisa;

- Istituto di Fisica Atomica e Molecolare del CNR, Pisa;

- Dipartimento di Chimica e Chimica Industriale dell' Università di Pisa;

- Dipartimento di Fisica dell'Università di Pisa;

- Scuola Normale Superiore, Pisa

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

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

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

E-mail: pisa2000@indigo.icqem.pi.cnr.it

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 ,

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

10. Faraday Discussion 117 - EXCITED STATES AT SURFACES

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

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

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

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

ORGANISING COMMITTEE

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

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

11. 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)

Special announcements

INVITATION TO SUBMIT A PAPER

The journal **Physical Chemistry Chemical Physics** (a merger of the Journal of the Chemical Society Faraday Transactions and Berichte der Bunsen-Gesellschaft für Physikalische Chemie from Jan. 1999) will publish articles in the area of "PHOTODYNAMICS FROM ISOLATED MOLECULES TO CONDENSED PHASES", in connection with the Havana Conference (n. 6, previous section).

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

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

BOOKS

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/>