Molecular Dynamics News

number 104; December 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 has been accepted - otherwise state *unpublished*).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 105 to Prof. V. Aquilanti. **(You are encouraged to use electronic mail: AQUILA@DYN.UNIPG.IT)**. (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#104). The closing date for issue number 105 is February 1, 2000.

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*2000 Calendar-Year subscription for **MDN**, (six issues).

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

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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:
join molecular-dynamics-news John F Kennedy
You do not need to tell the program your email address, as it picks it up from the message header. It does needs to be told your real name, so that it can maintain a useful list of email addresses.
When you join, you will receive some introductory information on how to circulate information to the molecular-dynamics-news list, and on the mailbase system itself.
If you would like a list of the current members, send a message containing the line
review molecular-dynamics-news
to the address mailbase@mailbase.ac.uk
Note that messages distributed via the e-mail list are not normally printed in the newsletter, unless the Editors receive an explicit request to do so.

a. Open Positions

FACULTY

Professorship in molecular and optical physics, Lyon, France

A professorship in molecular and optical physics is likely to become vacant at the Universite Claude Bernard, Lyon I (France), with a starting date October 2000.

The applicant will teach Optics, Laser Physics and Electromagnetism at undergraduate and postgraduate level.

The position will be associated with the Laboratoire de Spectromtrie Ionique et Moleculaire (LASIM) within the physics department. The laboratory wishes either to reinforce the existing molecular spectoscopy group of Professor J. d'Incan (retirement July 2000), using the high resolution Fourier transform spectrometry facility to work in atmospheric physics, or else to start a new independent research group in Optics, with interests in the non-linear properties of molecules at surfaces, in nanoparticles or aerosols. In the latter case, the new group will be expected to forge stronger links with the groups working on clusters, or on atmospheric pollution within the laboratory, and to interact with the nanotechnology projects of the physics department.

Informal enquiries should be addressed to:

Professor Michel Broyer (Directeur du Laboratoire)
Laboratoire de Spectrometrie Ionique et Moloculaire
Batiment 205, Universite Claude Bernard Lyon I
Campus La Doua, 69622 Villeurbanne Cedex
FRANCE
tel (33) 04 72 44 82 60, broyer@lasim.univ-lyon1.fr
or to Dr Christian Bordas, tel (33) 04 72 43 10 86, or to Dr Amanda Ross, tel (33) 04 72 44 85 63

REMINDER : Although this position will not be officially published until Spring 2000, the closing date for registration on the 'Liste de qualification aux fonctions de professeur aux universitas' has been set by the Ministere d'Education Nationale at 10th November 1999.

LECTURER (MAITRE-ASSISTANT) POSITION, UNIVERSITY OF LAUSANNE (SWITZERLAND)

A lecturer (maitre-assistant) position is available immediately at the Institut de Physique de la Matere Condense-University of Lausanne. The candidate is expected to take part in teaching advanced physics courses to third and fourth (final) year students and/or basic physics to first year pharmacy and medical students. He or she will be involved in a research project using ultrafast laser spectroscopy to study photoinduced dynamics in condensed phase chemical systems and in biological molecules. The candidate should have a PhD in Physics or Physical Chemistry, along with at least two years of postdoctoral experience in the field of Ultrafast Spectroscopy. Knowledge of french language is highly recommended but not a condition. The base salary is approx. SFr. 80'000.- per annum. The University of Lausanne offers the possibility to do a habilitation.

Please send CV, list of publications and 2 Letters of recommendation to:

Prof. Majed CHERGUI, Vice-chair
Institut de Physique de la Matiere Condensee
Faculte des Sciences, BSP
Universite de Lausanne
Ch-1015 Lausanne, Switzerland
tel.: xx-41-21-692 3678 (direct), (21) 692 3660 (secr.) Fax.:xx-41-21-692 3635, email:
Majed.Chergui@ipmc.unil.ch
http://WWW.UNIL.CH/ipmc/

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 Universite 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, Universite 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

DEPARTMENT OF CHEMISTRY, University of Southampton, UK
An EPSRC funded postdoctoral position is available to work with Dr Richard Moss. The salary will be from £ 17570 and the starting date is as soon as convenient.
The title of this theoretical project is ”Calculation of fully nonadiabatic properties of the hydrogen molecular cation and its isotopomers”. It will involve analytical and computational quantum mechanics.
Further details of the project are at
http://www.soton.ac.uk/∼chemweb/jobs/physchem/remoss2.html
and details of the Department may be found at
http://www.soton.ac.uk/∼chemweb
Dr Richard E Moss, Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK
Tel: +44 (0)23 80592193, FAX: +44 (0)23 80593781
email: rem@soton.ac.uk
www: http://www.soton.ac.uk/∼rem

POST DOCTORAL POSITION , University of Canterbury, New Zealand

Post Doctoral position with Professor Peter Harland and Dr Robert Maclagan, Chemistry Department, University of Canterbury, Private Bag 4800, Christchurch, NEW ZEALAND.

A Marsden Fund (New Zealand Government) Post Doctoral position is available from 1st March 2000 for up to 24 months to investigate the dynamics of ion and electron collisions with spatially oriented molecules by crossed particle beams. Experience in experimental chemical physics, preferably involving crossed molecular beam studies, would be an advantage. A working knowledge of ultra-high vacuum systems, computer interfacing of instrumentation and techniques used for the measurement of small signals is essential. Preference will be given to candidates with experience in one or more of the following areas: charged particle studies; ion-imaging; instrument design; and computational chemistry.

The project leaders maintain collaborative links with international research groups including Rice University, The University of Georgia and The University of Oxford.

Salary $NZD45,000 p.a. The average wage in New Zealand is $NZ35,000. The cost of living in Christchurch is substantially lower than for the U.S. or Europe and the Post Doctoral salary will allow the appointee and family to live comfortably.

Christchurch is a city of 325,000 with excellent sporting and cultural opportunities. The Chemistry Department is recognised as one of the top Chemistry Departments in the Southern Hemisphere. Information about the University is available on the web at http://www.canterbury.ac.nz/ and http://www.canterbury.ac.nz/campusinfo/about/intro.htm

Further information can be obtained from Professor Harland at the above address or p.harland@chem.canterbury.ac.nz

telephone: +64 3 364 2454 (Note that NZ time is GMT+12), fax: +64 3 364 2110

NRC Postdoctoral Openings, Hanscom Air Force Base

Two National Research Council Associate positions are available at the Air Force Research Laboratory at Hanscom Air Force Base, 15 miles northwest of Boston, Massachusetts. We perform laboratory research to better understand the chemistry and physics of the upper atmosphere. The research is conducted in an academic style and results are published in the open literature. U.S. citizenship is required for these positions, and applicants should be either soon-to-be or recent (past five years) PhD's. A modest-length proposal, written with input from an AFRL staff member, is due 15 Jan 2000 together with supporting documents. The position is nominally for one year, with a second year of funding contingent on mutual interest. Salary is about $45,000/year. See http://national-academies.org/rap for further details. We encourage submissions from motivated individuals, including those who wish to broaden their experimental knowledge base. Please contact the appropriate scientist (see below) for further information.

Position 1:Experiments in the COCHISE (COld CHemical Infrared Simulation Experiment) facility will be pursued, specifically: the spectroscopy and kinetics of excited nitrogen atom collisions with oxygen molecules [fast $N + O_2 \rightarrow NO(v, \text{high } J) + O$] The details of the very highly rotationally excited product states of NO will be investigated as a function of precursor state. Metastable species will be monitored using spectrometric and interferometric detection of visible and IR emissions. Please contact Dr. Steven Miller at 781.377.2807 or miller@plh.af.mil for further information.

Position 2:Experiments in the laser laboratory investigating energy transfer in key aeronomic processes will be pursued. Notably, these include vibrational energy transfer in collisions of NO and CO_2 with oxygen atoms. Laser techniques, including laser-induced fluorescence and transient diode laser absorption, will be used to detect the relevant species. Complex spectral and kinetic models will be developed to analyze and interpret the resultant data. Please contact Dr. Jim Dodd at 781.377.4190 or dodd@plh.af.mil for further information.

NRC Postdoctoral Opening, Hanscom Air Force Base

A National Research Council Associate position in theoretical Molecular Dynamics is available at the Air Force Research Laboratory (AFRL) at Hanscom Air Force Base, about 15 miles northwest of Boston, Massachusetts. We perform research to better understand the chemistry and physics of the non-equilibrium

upper atmosphere. The research is conducted in an academic style and results are published in the open literature (See The Journal of Geophysical Research A, Geophysical Research Letters, and Chem. Phys. Lett. for our recent work). U.S. citizenship is required for this position, and applicants should be either soon-to-be or recent (past five years) PhD's. A modest-length proposal, written with input from an AFRL staff member, is due 15 Jan 2000 together with supporting documents. The position is nominally for one year, with a second year of funding contingent on mutual interest. Salary is about $45,000/year. See http://national-academies.org/rap for further details. Please contact Dr. Ramesh Sharma at 781.377.4198 or sharma@plh.af.mil for further information.

Postdoctoral position, Hebrew University of Jerusalem

I am happy to announce an opening for a postdoctoral-position at the Hebrew University of Jerusalem, regarding Quantum Simulations of Proton Mobility and Acid Dissociation in water. This is a joint project with Prof. G.A. Voth, from the University of Utah, whose aim is to analyze in detail classical and quantal MD results obtained using the Utah MS-EVB/CMD software package, to elucidate the molecular mechanisms governing these fundamental processes.

Starting date: December 1999 in Jerusalem. Maximal duration – 3 years. A stay of several months in Salt Lake City during the year 2000 is anticipated. Fellowship is commensurate with regulations of the above Institutions and with candidate's qualifications, which should include: Good background in molecular dynamics, Fortran programming; Quantal calculations and parallel processing experience could be useful. Excellent/experienced Ph.D. candidates will also be considered. Kindly send updated CV, grades, list of publications and 2 letters of reference to:

Prof. Noam Agmon, Dept. Physical Chemistry, Givat-Ram Campus, The Hebrew University, Jerusalem 91904, ISRAEL

tel. 972-2-6585687, FAX 972-2-6513742, Email: agmon@fh.huji.ac.il

Homepage: www.fh.huji.ac.il/∼agmon/index.html

Postdoctoral position, University of Helsinki

A postdoctoral position is available in the Laboratory of Physical Chemistry, University of Helsinki, Finland for one year starting 1.1.2000. The monthly salary is about 2520 Euro (approx. 2650 USD). The successful candidate is expected to carry out experimental research in the field of laser spectroscopy, particularly developing new spectroscopic laser methods for molecular overtone state studies. For some of our publications see J. Chem. Phys. 110, 1424 (1999), Adv. Chem. Phys. 104, 41 (1998), J. Chem. Phys. 107, 1680 (1997); 104, 488 (1996); 102, 3911 (1995), Chem. Phys. Letters 219, 181 (1994), J. Chem. Phys. 99, 3277 (1993), Rev. Scient. Instr. 63, 5546 (1992), Chem. Phys. Letters 189, 205 (1992). The Helsinki molecular spectroscopy group has excellent experimental facilities and it does both experimental and theoretical work. The group consists of about 10 people. More information can be obtained from Prof. Lauri Halonen, tel. +1-303-492-8046, fax +1-303-492-5235, e-mail halonen@jila.colorado.edu , home page http://fkassistant.pc.helsinki.fi/

Please send the applications to the address: Prof. Lauri Halonen, JILA, University of Colorado at Boulder, Campus Box 440, Boulder, Colorado 80309-0440, USA. The closing date is 22nd November 1999.

Camille & Henry Dreyfus Postdoctoral Fellowship, Boston College

A Camille & Henry Dreyfus Postdoctoral Fellowship is available to perform atmospheric chemistry laboratory studies in a joint program conducted in the Department of Chemistry at Boston College and at Aerodyne Research Inc. The research focuses on the heterogeneous interactions of atmospherically important gas phase species with liquids and with submicron aerosols, 40 to 1000 nm in diameter. Gas-liquid interactions are studied in droplet and bubble train apparatuses. Aerosol experiments are performed in a new apparatus that couples an aerosol sampling mass spectrometer with a fast flow reactor. The goal of the work is the study of chemical reactions of gas phase species with liquids and aerosols. The aerosol experiments are also designed to study changes in physical size and chemical composition of the aerosols after controlled exposure to reactive trace gases. The person in this position will participate in the on-going development of this novel apparatus as well as in the experimental studies. Experience in vacuum techniques and mass

spectroscopy is desirable. This postdoctoral position presents an opportunity to be introduced to important aspects of atmospheric chemistry. Applicants should send their vita to Prof. Paul Davidovits, Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill MA 02467, e-mail: paul.davidovits@bc.edu , Phone 617-552-3617. Boston College is an Equal Opportunity/Affirmative Action employer.

NRC Postdoctoral Opening, Hanscom Air Force Base

The Space Chemistry group of the Air Force Research Laboratory Space Vehicles Directorate at Hanscom AFB. MA, is looking to fill an NRC post-doctoral research associate position. The successful candidate will conduct experimental research on ion processes using guided-ion beam and photodissociation techniques. Projects include the study of hyperthermal chemistry of atmospheric ions with small organic molecules, ion-metal vapor chemistry, inelastic and elastic scattering of atomic ions with atoms, photodissociation dynamics of small cluster ions, and the collision-induced dissociation dynamics of diatomic ions at high levels of vibrational excitation. The latter project is a collaborative effort with Prof. C. Y. Ng and involves prolonged assignments at the Lawrence Berkeley Advanced Light Source. The conducted research applies to modeling of extreme environments such as those of reentry vehicles, meteors, and electric propulsion spacecraft thrusters.

The National Research Council (NRC) Resident Research Associateship Program provides highly qualified and motivated individuals AFRL on-site research assignments for one year, with second and third year extensions possible.

More information regarding the NRC associateship program can be obtained at the website, http://www4.nationalacademies.org/osep/rap.nsf or by calling Ms. Jacinta Kelly 202-334-1423.

Interested candidates should contact:

Rainer A. Dressler, Air Force Research Laboratory, AFRL/VSBS, 29 Randolph Rd, Hanscom AFB, MA 01731-3010

Tel: 781-377-2332, Fax: 781-377-8202, Email: Dressler@plh.af.mil

World Wide Web: http://www.plh.af.mil/Star/CPSE

Postdoctoral Position, University of Utah

A postdoc position is available in the lab of Scott Anderson, starting anytime after 1 January, 2000. The postdoc will work on our mode-selective ion-molecule reaction experiment, studying the reaction dynamics of simple polyatomic systems. We use REMPI and MATI ionization to prepare cations with variable excitation in selected vibrational modes, then study reactions in a high resolution guided-ion beam machine. The instrument also allows measurements of product velocity and angular distributions. Vibrational effects probe the early part of the collision, up to the point of initial ”impact”. The nature of the types of reactant motion (vibrational mode and relative energy) provide insight into the factors (e.g. transition state structure) that control reactivity and product branching. Angular distributions, coupled with isotope labeling, provide a measure of the timescale of the collisions, and how this varies with reactant energy and state. In direct reactions, the angular information allows us to distinguish between scattering mechanisms, and indirectly provides insight into the impact parameter dependence of the reactivity and product branching. Additional information can be found at my web site (see below) under the ”State-selective Ion Chemistry” link. Experience with pulsed laser spectroscopy and vacuum systems is desirable, however, I am most interested in working with a creative experimentalist. The initial appointment will be for one year, with the expectation of renewal for a second year contingent upon reasonable progress. Salary will be competitive, and the position includes excellent health insurance. Salt Lake is a great place to live, with world-class skiing, hiking, and biking close by, good neighborhoods near campus, and excellent public schools. The University of Utah is an AA/EEO employer, and applications from qualified women and minority candidates are encouraged. If interested, please send a C V and arrange for three letters of recommendation to be sent to:

Scott L. Anderson, Professor of Chemistry, Dept. of Chemistry, 315 S. 1400 E., University of Utah, Salt Lake City, UT 84112-0850

(801) 585-7289, (801) 581-8433 FAX, www.chem.utah.edu/chemistry/faculty/anderson/anderson.html

Postdoctoral position, Leiden University

A post-doc position is available in the group of Geert-Jan Kroes at Leiden University, starting anytime after 1 January 2000, for a total period of two years.

The post-doc will do research on the quantum dynamics of a gas phase four-atom reaction that is a paradigm for reactions that proceed through the formation of a long-lived collision complex. Calculations will be attempted in which all six degrees of freedom are treated quantum mechanically, for total angular momentum J=0. For the system to be tackled, such calculations still represent a great challenge. In the calculations, a hybrid method will be used: the time-dependent wave packet method will be employed for the short time dynamics, which will be extrapolated to long times using information concerning resonances that is obtained with filterdiagonalization. The potential energy surface that will be used in the dynamics calculations is already available. Questions that will be considered are: (i) how does the formation of long-lived collision complexes affect the reactivity?, and (ii) does the bond that is not broken in the reaction act as a spectator? In the project, we will collaborate with Prof. D. Neuhauser (University of California at Los Angeles).

Scientists with a Ph.D. in Chemistry, Physics, or numerical Mathematics who are interested in molecular quantum mechanics and have experience with numerical methods and computer programming are asked to apply. The total salary (before taxes) will be between dfl 5153,- and dfl 8682,- per month, depending on experience. The appointment will be for two years.

Leiden is a pleasant town which is only half an hour away from Amsterdam by train, and Leiden University is the oldest and perhaps the most famous university of the Netherlands. The theoretical chemistry group of Marc van Hemert and Geert-Jan Kroes at Leiden is a lively and growing group which includes at present 1 post-doc and five graduate students, with one additional vacancy for a graduate student which will be advertized soon.

If interested, please send a letter and CV by airmail to the below address, and arrange for two letters of recommendation, to be sent as well to the below address (please use ordinary or air mail, not e-mail). The deadline for receiving letter and CV is 1 December 1999.

G.J.Kroes (geertj@rulgle.Leidenuniv.nl), LIC, Gorlaeus Laboratoria, Rijksuniversiteit Leiden, Postbus 9502, 2300 RA Leiden, The Netherlands

(tel.+31 71 527 4396, Fax (new number) +31 71 527 4488)

Postdoctoral Research Associate, University of Surrey

A 3-year Research-Council funded Postdoctoral Research Assistantship in Quantum Chemistry is available for work with Prof Graham A Webb and Dr Peter B Karadakov on the

Ab Initio Calculation of Spectroscopic Parameters Relevant to the Determination of Carbohydrate Polymer Structures.

Applicants should have a PhD in theoretical chemistry or chemical physics; previous experience with ab initio codes such as GAUSSIAN and GAMESS is also desirable.

Starting salary will be on the RA1A scale in the range 16,286-19,869 per annum according to age and experience.

Further information can be obtained from:

Prof Graham A Webb (e-mail: g.webb@surrey.ac.uk) or

Dr Peter B Karadakov (e-mail: p.karadakov@surrey.ac.uk)

Department of Chemistry, University of Surrey, Guildford, Surrey GU2 5XH, UK

tel +44 (0)1483 876828—fax +44 (0)1483 876851

Applications should be accompanied by a CV and the names and addresses of two referees.

POSTDOCTORAL POSITION, UNIVERSITY OF NORTH CAROLINA

We are looking for a post-doc interested in moving into the emerging field of aerosol chemistry. This position will be joint between the research groups of Tom Baer and Roger Miller, on an AFOSR funded project dealing with the laser initiated combustion of single aerosol particles. The apparatus consists of a TOF laser-mass spectrometer into which we inject aerosol particles. These are detected by light scattering from two green diode lasers. This provides the triggering for a CO2 laser, used to ”ignite” the particles and

for both a YAG pumped system and an excimer laser. The goal is to study the formation of radical intermediates during the liquid state combustion of these particles. A VUV laser is being developed to carry out near threshold ionization and H atom detection. REMPI and LIF is also available for state selective probing of the products, from which temperatures can be determined for the vapor plume. To date we have observed NO2 elimination from nitrotoluene. We are now carrying out studies on higher energy molecules that can give rise to auto-catalytic processes.
This apparatus will also be used to determine compositions of atmospheric aerosols, related to the PM2.5 issues. Ultimately we would like to develop methods that would enable us to depth profile such particles, providing detailed test of the molecules for organic aerosols and opening up a whole new range of uptake experiments.
The candidate need not have experience in aerosol science, but rather should have expertise in pulsed laser, TOF mass spectrometry.
Please send a cv and two letters of recommendation to: Tom Baer or Roger Miller, Chemistry Department, CB# 3290 Venable Hall, Chapel Hill, NC 27599-3290

POSTDOCTORAL POSITION, NATIONAL RESEARCH COUNCIL OF CANADA, OTTAWA
We would like to hire a postdoctoral fellow in the area of theoretical molecular chemical physics. Experience in ab initio electronic structure calculations and/or variational and perturbative calculation of rotation-vibration energies would be an asset. We provide the successful applicant with a single node SGI 2000 workstation, and the Theory Group shares a 108 node SGI ORIGIN 2000.
Phil Bunker's research interests and recent publications can be viewed at http://www.sao.nrc.ca/∼bunker
Application can be made by clicking on "NRC Post-Doctoral Fellowship" at the site
http://hr.nrc.ca:8080/HRB/CareerPg.nsf/GradE
If you apply please also contact Philip.Bunker@nrc.ca

POSTDOCTORAL POSITION, IMPERIAL COLLEGE, LONDON
Applications are invited for a post-doctoral position, to join a team developing and applying new two dimensional non-linear spectroscopic techniques to the study of condensed phase chemical and biochemical systems.
Candidates should ideally have experience in the application of ultra-fast spectroscopic techniques for the study of condensed matter systems, however given the cross-disciplinary nature of the research group, strong candidates from related disciplines are also encouraged to apply.
The position is for up to three years, with salary ranging from £ 16,286 - £ 24,479 plus £2,134 London allowance.
Applications including CV and letters of reference, or requests for further information, should be sent to:
Dr Ian Mercer, Chemistry, Imperial College, South Kensington. London. SW7 2AY. UK.
Phone/ans.phone/fax: +171 594 5828 Email: i.mercer@ic.ac.uk
Closing date for applications: 10th December 1999.

POSTDOCTORAL POSITIONS, NATIONAL RESEARCH COUNCIL OF CANADA, OTTAWA
Two postdoctoral positions are available in my group at the National Research Council in Ottawa.
We are currently pursuing theoretical research in several areas of molecular dynamics including:
* Gas-surface interactions: Control of surface reactions using a scanning tunneling microscope.
* Photomanipulation of external molecular modes: Molecular optics and molecular alignment with intense laser fields. [For recent publications in this area see: Phys. Rev. Lett. **83** (Dec. 6, 1999); J. Chem. Phys. **111**, 4397 (1999); J. Chem. Phys. **111**, 4113 (1999); J. Chem. Phys. **108**, 6272 (1998); J. Chem. Phys. **107**, 10429 (1997); Phys. Rev. A **56**, R17 (1997); J. Chem. Phys. **106**, 2881 (1997).]
* Time-resolved photoelectron spectroscopy as a probe of ultrafast, electronically nonadiabatic processes and of rotation-vibration coupling mechanisms. [Nature **401**, 5 (1999); J. Chem. Phys. **110**, 147 (1999); J. Chem. Phys. **107**, 7859 (1997).]
* Molecular interferometry in configuration space: The application of coherent control techniques to explore molecular continua. [J. Chem. Phys. **111**, 9168 (1999); Faraday. Discuss. **113**, 61 (1999); Accts. Chem.

Res., **32** (Dec. 1999); Phys. Rev. Lett. **82**, 65 (1999); J. Chem. Phys. **108**, 1915 (1998); Phys. Rev. Lett. **79**, 4108 (1997).]
For more details and for abstracts of submitted papers and papers in press see: http://gold.nrc.ca/∼tamar
or contact me at: tamar.seideman@nrc.ca
The Steacie Institute of the National Research Council offers multi-disciplinary research and a collaborative atmosphere. My group is lively and international and the computational facilities are excellent.
Applicants are asked to send me their Curriculum Vitae and to have two or more letters of recommendation sent to me directly, either by e-mail or by regular mail.

POSTDOCTORAL POSITION, University of Alberta
A postdoctoral position is available in the group of Pierre-Nicholas Roy at the University of Alberta, Edmonton, Canada.
Research interests include the development of simulation methodologies for quantum molecular dynamics using path integral and semi-classical approaches.
Experience with classical and quantum molecular dynamics simulation methods is desirable. Candidates with a knowledge of parallel programming techniques are also strongly encouraged to apply.
Our computational resources include a 17 node PIII-500 Beowulf cluster and an IBM RS/6000 43P260 dual processor visualization workstation.
The starting date is early 2000 and the initial appointment is for a period of one year, renewable for another year (subject to the availability of funds).
Interested candidates should send a C.V., a summary of research interests and arrange for three letters of recommendation (email is ok) to be sent to Pierre-Nicholas Roy at the address below:
Professor Pierre-Nicholas Roy, Department of Chemistry, University of Alberta Edmonton, AB, Canada, T6G 2G2
tel: (780) 492-0317, fax: (780) 492-8231, email: pn.roy@ualberta.ca
www: http://www.chem.ualberta.ca/faculty/Physical/roy.htm

POSTDOCTORAL FELLOWSHIP, NATIONAL TSING HUA UNIVERSITY, TAIWAN
One postdoctoral position starting January 2000 is open at the Department of Chemistry, National Tsing Hua University, Hsinchu, TAIWAN. The candidate is expected to be involved in the application of step-scan time-resolved Fourier-transform spectroscopy to gas phase absorption of transient species. This is a new technique with great potential. Please refer to J. Chem. Phys. **107**, 6499 (1997) for related articles. The appointment is renewable yearly with a salary about US$24K plus housing. The tax is about 6% for those who stay more than 6 months in a calendar year. Applicants should send their c.v. and arrange 2-3 letters of recommendation to Prof. Yuan-Pern Lee, Department of Chemistry, National Tsing Hua University, TAIWAN 30043. (e-mail: yplee@mx.nthu.edu.tw , FAX: 886-3-5722892).

Postdoc Position, Hebrew University of Jerusalem
A postdoctoral position is available in the group of Roi Baer at the Hebrew University of Jerusalem, Israel.
In our group, we are developing an exciting new approach to quantum chemistry, using a new Quantum Monte Carlo Technique called ”Shifted Contour Auxiliary Field Quantum Monte Carlo”. (See references at bottom). This work is made in collaboration with Daniel Neuhauser from UCLA.
The method is exciting because it alleviates the fixed node errors of other quantum Monte Carlo methods and it allows correlated sampling of energetical differences.
Our computational resources include a 85 node PIII-500 MOSIX cluster. The appropriate candidate should have a strong background in programming and theoretical chemistry. Preference to candidates with experience using plane wave methods and experience in programming in C++. The starting date is immediate and the initial appointment is for a period of one year, renewable for another year (subject to the availability of funds).
Interested candidates should send a C.V., a summary of research interests and arrange for three letters of recommendation (email is ok) to be sent to Roi Baer at the address below.
References:

1) R. Baer, M. Head-Gordon and D. Neuhauser, ”Shifted-contour auxiliary field Monte Carlo for ab initio electronic structure: Straddling the sign problem” J. Chem. Phys.109, 6219 (1998).
2) R. Baer and D. Neuhauser, ”Molecular electronic structure using auxiliary field Monte Carlo, plane waves and pseudopotentials” J. Chem. Phys. (in press, 1999).
Both reprints and a slide show can be viewed or downloaded from: http://www.fh.huji.ac.il/∼roib/qmc.htm
Dr. Roi Baer, Dept. of Physical Chemistry and The Lise Meitner Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel
Tel: 972-2-658-6114, Fax: 972-2-651-3742 email: roib@fh.huji.ac.il
Web: http://www.fh.huji.ac.il/∼roib

Postdoctoral Position, Korea Advanced Institute of Science and Technology

We would like to control the branching ratio of the unimolecular dissociation of alkali dimers. The final goal would be the control of the reaction paths of bimolecular reactions. When the continuum is coupled with discrete states, asymmetric line profiles appear due to mutual interference. The product branching ratio can be changed abruptly along these asymmetric line profiles. We apply two coherent laser pulses and control the brancing ratios by adjusting the relative phase betrween the two laser fields. In order to apply complex excitation scheme, appropriate excited states are searched.
Recent Ph. D’s who have experience in laser spectroscopy and/or molecular beam are welcome. Our system is pulsed molecular beam of alkali metal dimers. We use Resonance Enhanced Multiphoton Ionization spectroscopy. Detection method by LIF would be utilized, too.
Theoreticians interested in ab initio calculation of alkali metal dimers can be considered for this position.
If you want more information please get to http://www.chem.kaist.ac.kr/Bongsoo_Kim.html
Professor Bongsoo Kim, Department of Chemistry, Korea Advanced Institute of Science and Technology, Taejon, Korea

THREE POSTDOCTORAL POSITIONS, BROOKHAVEN NATIONAL LABORATORY

The Gas-Phase Molecular Dynamics (GPMD) group in the Chemistry Department of Brook-haven National Laboratory, Upton, NY (USA) is a highly interactive, multidisciplinary team of researchers working on basic problems in spectroscopy, dynamics and kinetics related to obtaining a fundamental understanding of combustion processes at the molecular level (see http://www.gpmd.bnl.gov). The members of the group are:
James T. Muckerman (theoretical dynamics, spokesperson)
Trevor J. Sears (high-resolution absorption spectroscopy)
Gregory E. Hall (molecular dynamics using Doppler lineshape analysis)
Jack M. Preses (vibrational energy transfer)
Christopher Fockenberg (chemical kinetics).
Three postdoctoral positions are currently available for recent Ph.D.s: one in the area of theoretical/computational dynamics under the supervision of Dr. Muckerman; another in experimental chemical kinetics under the primary supervision of Dr. Fockenberg; and the other in experimental chemical dynamics under the supervision of Dr. Hall. The appointments are for one year, renewable for a second year, at an annual salary of approximately $31,000. Brookhaven National Laboratory (BNL) is an equal opportunity employer, and US citizenship is not required.
The successful candidate for the theoretical/computational dynamics position should have a strong background in quantum dynamics and scattering theory, and will participate in computational studies of the vibrational structure of small hydrocarbon radicals, the calculation of rate constants for chemical reactions from the cumulative reaction probability, and laser control of molecular motion. One facet of this research involves the development of computer codes that make efficient use of massively parallel architectures.
The successful candidate for the experimental chemical kinetics position should have a strong background in chemical kinetics or chemical dynamics, and will participate in kinetics studies on radical-radical chemical reactions involving small hydrocarbon radicals using a new apparatus with TOF mass spectrometry as its primary detection technique. The research also includes investigations with a diode laser absorption system on selected reactions.

The successful candidate for the position in chemical dynamics should have a strong background in laser spectroscopy or chemical dynamics and will perform experiments using Doppler-resolved transient FM laser spectroscopy. In recent years our group has developed and applied this technique to a variety of problems in photoinitiated unimolecular reactions and direct photodissociation. We plan to extend previous work on correlated state distributions and fragment polarization in unimolecular reactions as an experimental probe of the limits of validity for statistical theories of unimolecular reaction rates.
Applicants should submit a CV with a list of publications, a brief statement of research interest, and three letters of recommendation. Send all correspondence to:
James T. Muckerman (Email: muckerma@bnl.gov), or Christopher Fockenberg (Email: fknberg@bnl.gov), or Gregory E. Hall (Email: greghall@bnl.gov)
Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

Postdoctoral Position, National Research Council, Ottawa
A joint postdoctoral position in the area of time-resolved dynamics is available in the groups of Tamar Seideman and Albert Stolow at the Steacie Institute for Molecular Sciences of the National Research Council of Canada.
We are particularly interested in nonadiabatic dynamics in polyatomic systems as viewed by time-resolved photoelectron angular and energy distributions. The successful candidate will carry out theoretical work in the group of Tamar Seideman in direct collaboration with the experimental group of Albert Stolow.
Relevant recent Publications include:
1) V. Blanchet, M. Zgierski, T. Seideman and A. Stolow, ”Discerning Vibronic Molecular Dynamics via Time Resolved Photoelectron Spectroscopy”, Nature **401**, 52 (1999).
2) S.C. Althorpe and T. Seideman, ”Molecular Alignment from Femtosecond Time-Resolved Photoelectron Angular Distributions: Non Perturbative Calculations on NO”, J. Chem. Phys. **110**, 147 (1999).
3) V. Blanchet A. Stolow, ”Nonadiabatic Dynamics in Polyatomic Systems Studied by Femtosecond Time-Resolved Photoelectron Spectroscopy”, J. Chem. Phys. **108**, 4371 (1998).
4) T. Seideman, ”Time-Resolved Photoelectron Angular Distributions: A Nonperturbative Theory”, J. Chem. Phys. **107**, 7859 (1997).
For more details see:
http://gold.nrc.ca/∼tamar
http://gold.sao.nrc.ca/sims/femto_e.html
Or contact us at: tamar.seideman@nrc.ca or albert.stolow@nrc.ca

Postdoctoral Position, Concordia University
A postdoctoral position is available immediately in Computational and Theoretical Chemistry in the Department of Chemistry and Biochemistry at Concordia University. The successful candidate will be involved in various components of our research program, including studies of novel cluster materials and catalysts, cluster and liquid solvation in photochemistry, proton transfer and role of hydrogen bonding in biological systems. Preference will be given to candidates with a strong background in traditional, Car-Parrinello and QM/MM Molecular Dynamics Simulations, and/or Electronic Structure Calculations. Solid programming ability a plus. Salary commensurate with experience. Fax, mail or e-mail letter of intent and resume, and have three reference letters sent to Prof. Gilles H. Peslherbe, Department of Chemistry and Biochemistry, Concordia University, 1455 De Maisonneuve Blvd West, Montreal, Quebec, CANADA H3G 1M8. Fax: (514) 848-2868. E-Mail: ghp@alcor.concordia.ca . More information can be found at http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe .
Professor Gilles H. Peslherbe, Concordia University, Department of Chemistry and Biochemistry, 1455 De Maisonneuve Blvd Ouest, Montreal, Quebec, CANADA H3G 1M8
Tel: (514) 848-3335, Lab: (514) 848-3336, Fax: (514) 848-2868, E-Mail: ghp@alcor.concordia.ca
http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe

Postdoctoral Research Assistantship, University of Bristol
Applications are invited for a Postdoctoral Research Assistantship to work for up to 2 years with Dr Colin Western on the development of a novel, very high resolution, all solid state pulsed laser system and its application to the spectroscopy and dynamics of molecular systems. Applicants should have a PhD in either Chemistry or Physics. The position, which would particularly suit persons with a background in laser development or laser spectroscopy is available from 1 April 2000. Salary will be on the RA1A scale, currently in the range £16,286 - £18,185 pa.
Informal enquiries should be directed to: C.M.Western@bristol.ac.uk or see:
http://www.chm.bris.ac.uk/pt/western/vac2.htm
For further details telephone (0117) 954 6947, minicom (0117) 928 8894 or E-mail Recruitment@bris.ac.uk quoting reference 6046. 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 by the 21 Jan 2000.

POSTDOCTORAL POSITION, BROOKHAVEN NATIONAL LABORATORY
A postdoctoral position is available in chemical dynamics involving thermal and photo-induced reactions of adsorbates on metal and metal-oxide surfaces.
State-resolved probes of the desorbed products are used to study the charge and energy transfer processes induced by photoexcitation at the adsorbate-metal interface and the resulting reaction dynamics leading to desorption. Current and future projects include fundamental studies of photodesorption, UV and IR-induced recombination and association reactions, surface reaction kinetics and molecular beam scattering. This work is part of a larger interdisciplinary surface chemistry effort at BNL which includes access to spectroscopy and structural beam lines at the National Synchrotron Light Source.
The successful candidate should have a strong background in laser-based chemical dynamics, surface (photo)chemistry or surface scattering. Experience with REMPI techniques, time-of-flight mass spectrometry or ion-imaging is also desirable. Brookhaven National Laboratory is an equal opportunity employer, and US citizenship is not required.
Applicants should send a CV and three letters of recommendation to:
Michael G. White, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973
ph: (516) 344-4345, fax: (516) 344-5815, e-mail: mgwhite@bnl.gov

POSTDOCTORAL POSITION, UNIVERSITY OF PERUGIA
Applications are invited for a postdoctoral fellowship in Astrophysical Chemistry under the supervision of Professor Piergiorgio Casavecchia, and funded by the European Union's TMR (Training and Mobility of Researchers) Programme, as part of the TMR Network on "Astrophysical Chemistry: Experiments, Calculations, and Astrophysical Consequences of Reactions at Low Temperatures". This programme involves eight laboratories: University of Birmingham (UK), University College London (UK), University of Goettingen (Germany), Technische Universitat Chemnitz (Germany), University of Rennes (France), Observatoire de Paris, Meudon (France), University of Bordeaux (France), and the University of Perugia (Italy).
The focus in our laboratory is on studies of chemical reaction dynamics using the Crossed Molecular Beams scattering technique with universal mass-spectrometric detection. Investigation of elementary atom(radical)-molecule and atom-radical reactions of relevance to Astrochemistry are being pursued. We exploit the novel capability of generating intense and continuous supersonic beams of carbon and nitrogen atoms, and hydroxyl (OH) and cyano (CN) radicals. All these beams have already been successfully tested and used for experiments. Experiments are planned on N, C, and CN reactions, as well as on atom-radical reactions as N+OH. More details of the research field, the technique used, and publications may be found at the following site: http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html and details of the Astrophysical Chemistry TMR Network should also be consulted: http://www.bham.ac.uk/Astrochemistry/
The position is available from January 2000 for one year (actually 13 months). The exact commencement date is negotiable. The post-doc is expected to spend up to one month each year in another laboratory of the TMR network. Salary is about 3000 EURO/month. 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., Italy) and must not have carried out their normal activities in that state for more than 18 of the 24 months prior to their appointment. Experience in reaction dynamics and molecular beams is desirable.
Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcomed. Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universita di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

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) 996-043, 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-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, H_2SO_4, 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 in 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 Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan

A postdoctoral position is available in my group in the Institute of 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 HO_2 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

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://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:
The University of Waterloo, which has nore 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.UWwaterloo.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

b. Preprints

Chemical reaction dynamics with molecular beams
Reports on Progress in Physics
P. Casavecchia
Dipartimento di Chimica, Universita di Perugia, 06123 Perugia , Italy piero@dyn.unipg.it
This comprehensive review describes advances which have occurred during the past decade in chemical reaction dynamics using crossed molecular beams and laser techniques.

The dynamics of the reaction Cl + $H_2(D_2)$ $\rightarrow$ HCl(DCl) + H(D): A Crossed beams, quasiclassical trajectory, and quantum mechanical scattering study
Phys. Chem. Chem. Phys. (submitted)
M. Alagia, N. Balucani, L. Cartechini, P. Casavecchia*, and G.G. Volpi
Dipartimento di Chimica, Universita di Perugia, 06123 Perugia , Italy piero@dyn.unipg.it
F.J. Aoiz* and L. Barares
Departamento de Quimica Fisica, Facultad de Quimica, Universidad Complutense, 28040 Madrid, Spain
T.C. Allison, S.L. Mielke, and D.G. Truhlar*
Department of Chemistry, Chemical Physics Program, and Supercomputer Institute, Univeristy of Minnesota, Minneapolis, MN 55455-0431, USA

Cyanomethylene formation from the reaction of excited nitrogen atoms with acetylene: a crossed beam and ab initio study
J. Am. Chem. Soc. (submitted)
N. Balucani, M. Alagia, L. Cartechini, P. Casavecchia*, and G.G. Volpi
Dipartimento di Chimica, Universit di Perugia, 06123 Perugia , Italy
piero@dyn.unipg.it
K. Sato
Department of Applied Physics, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo, 152- 8551, Japan
T. Takayanagi and Y. Kurosaki
Advanced Science Research Center, Japan, Atomic Energy Research Institute, Tokaai-mura, Nakagun, Ibaraki, 319-1195, Japan.

Comparative dynamics of Cl(^{2}P) and O(^{2}P) interactions with a liquid hydrocarbon surface
J. Chem. Phys. (submitted)
D.J. Garton, T.K. Minton*
Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT 59717, USA

M. Alagia, N. Balucani, P. Casavecchia, and G.G. Volpi
Dipartimento di Chimica, Universit di Perugia, 06123 Perugia , Italy piero@dyn.unipg.it
The dynamics of the interactions of atomic chlorine with the surface of a saturated hydrocarbon liquid, squalane, were investigated by directing supersonic beam of Cl atoms onto the squalane surface and by detecting the volatile products, Cl and HCl, using mass spectrometry as a function of incident angle, final angle, and incident Cl-atom energy. The results are compared to those of an earlier study on analogous oxygen-atom interactions.

Quasiclassical trajectory study of the H + CIF → F+ HCl, Cl + HF and F + HCl → Cl + HF reactions and their deuterium isotope variants on a new (2 A') ab initio potential energy surface
Phys. Chem. Chem. Phys. (Special Issue dedicated to Prof. R.Grice)
R. Sayos a) *, J. Hernando a) , R. Francia b) , and Miguel Gonzalez a) *
a) Departament de Quimica Fisica, Universitat de Barcelona, Marti i Franques, 1, 08028 Barcelona, Spain.
b) Departamento de Quimica, Universidad de La Rioja, Obispo Bustamante, 3, 26004 Logroo, Spain
In this work we present a quasiclassical trajectory study of the title reactions (with H or D) on a recent ab initio ground 2A' PES, mainly for reactants at 300 K. Rate constants, vibrational and rovibrational distributions, angular distributions and mean energy fractions disposed into products were analyzed and agreed well with available experimental data. The H + CIF → Cl + HF reaction exhibited a double microscopic: direct or migratory plus insertion, which gave place to very different reaction attributes for each mechanism.

Quantum Solutions for the Harmonic Parabola Potential System Physical Review A
K. H. Yeon, S. Zhang, Y. D. Kim, C. I. Um and Thomas F. George*
Office of the Chancellor / Departments of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897 tgeorge@uwsp.edu
This system is analyzed and applied to the cases of a quantum well, barrier and periodic lattices, where for the last case dispersion relations, energy states and bands are obtained.

Reply to 'Comment on Exact Wave Function of a Harmonic Plus an Inverse Harmonic Potential with Time-Dependent Mass and Frequency'
Physical Review A
C. I. In Um, S. M. Shin, K. H. Yeon and Thomas F. George*
Office of the Chancellor / Departments of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897 tgeorge@uwsp.edu
The exact wave function is obtained by a canonical and unitary transformation and the Lewis-Risenfeld invariant method.

Oxide Layer Growth Dynamics Induced by Lasers
Internation Journal of Theoretical Physics, Group Theory, and Nonlinear Optics
L. Fabian, Cs. Beleznai, R. Vajtai, D. Vouagner, Thomas F. George* and L. Nanai
Office of the Chancellor / Departments of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897 tgeorge@uwsp.edu
Effects due to a CW IR laser, to a pulsed UV laser and to their simulaneous use are presented.

Linear and Nonlinear Optical Susceptibility of Maxwell Garnett Composites: Dipolar Spectral Theory
Physical Review B
M. I. Stockman, K. B. Kurlayev and Thomas F. George*
Office of the Chancellor / Departments of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897 tgeorge@uwsp.edu
The linear dielectric constant and third-order hyperpolarizability are obtained for disordered composites consisting of nanospheres in a dielectric host.

Some Theoretical and Numerical Approaches to the Optics of Fractal Smoke
Optics of Nanostructured Materials, edited by V. A. Markel and T. F. George (Wiley-Interscience, New York)
V. A. Markel, V. M. Shalaev and Thomas F. George*

Office of the Chancellor / Departments of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point, Stevens Point, WI 54481-3897 tgeorge@uwsp.edu
Focusing on the purely electromagnetic problem, fluctuations of the light intensity scattered by random smoke aggregates and the absorption of light by smoke clusters places inside water microdroplets are considered in the first Born approximation.

c. Conferences

1. 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,...)

2. 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

3. 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 Laussanne, 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 preregistration 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 Tecnologoa 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

4. CONDENSED MATTER DIVISION, EUROPEAN PHYSICAL SOCIETY

Montreux, Switzerland, March 13 to 17, 2000

The next (18-th) General Conference of the Condensed Matter Division of the European Physical Society will be held in Montreux, Switzerland from March 13 to 17, 2000, jointly with the Japanese and the Swiss Physical Societies (see http://www.eps-cmd18.ch for details). The Conference consists of plenary sessions, parallel sessions and 1/2 day mini-colloquia on specialised topics. A mini-colloquium (see abstract below) will be organized on

ULTRAFAST SPECTROSCOPY OF CONDENSED MATTER
and will contain invited talks, contributed oral presentations and poster presentations.
The invited speakers are:
Jochen FELDMANN, Univ. Muenchen, Germany
Soren KEIDING, Univ. of Aarhus, Denmark
Takayoshi KOBAYASHI, Univ. of Tokyo, Japan
We strongly encourage you to submit abstracts for contributed papers and for posters. Abstracts should be submitted via the Web page of the conference http://www.eps-cmd18.ch before November 15th, 1999. Please fax or email a copy to M. Chergui (see address below).
IMPORTANT DEADLINES: 15 November 1999 Abstract submission
31 January 2000 Conference registration
21 February 2000 Hotel registration
M. Chergui, V. Sundstrom (Villy.Sundstrom@chemphys.lu.se) Chairs of the mini-colloquium
MINI-COLLOQUIUM ON ULTRAFAST SPECTROSCOPY OF CONDENSED MATTER
The scope of the mini-colloquium is to present the most recent scientific and technological developments in the field of ultrafast spectroscopy. In addition to the traditional condensed matter systems which are being investigated by ultrafast spectroscopy (e.g. semi-conductors), ultrafast phenomena in many body systems such as clusters, solutions, surfaces and interfaces, molecular solids and biological systems will be covered. The phenomena of interest include carrier dynamics, structural dynamics, energy dissipation, energy transfer, electron dynamics, chemical dynamics and solvent dynamics. From the technological point of view, the development of new ultrashort light sources from the IR to the X-ray domain will be covered, as well as new experimental techniques for the study of condensed matter. The mini-colloquim will include 3 invited talks, 6 to 8 contributed talks and a 2-hour poster session.

5. FARADAY DISCUSSION 115 - MOLECULAR PHOTOIONISATION
The University of York, 3-5 April 2000
The Faraday Discussion page (York): http://rempi.york.ac.uk/rscconf.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

6. 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	Nadine HALBERSTADT
Philippe.Brechignac@ppm.u-psud.fr	nhalbers@irsamc1.ups-tlse.fr
Labo. Photophysique Moleculaire	Labo. Physique Quantique, IRSAMC
Universite de Paris-Sud	Universite Paul Sabatier
Bat. 210	118, route de Narbonne
F 91405 ORSAY CEDEX, France	31062 - TOULOUSE CEDEX, France
Tel. +33 (0)1 69 15 67 79	Tel: +33 (0)5 61 55 64 88
+33 (0)1 69 15 67 76 (secr.)	+33 (0)5 61 55 68 34 (secr.)
Fax +33 (0)1 69 15 67 77	Fax: +33 (0)5 61 55 60 65

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

7. DYNAM 2000: Satellite Meeting of the Xth ICQC on Chemical Dynamics

Arcachon, France, 31 May - 3 June 2000 (just before the International Conference on Quantum Chemistry, Xth ICQC, in Menton

This meeting will cover the theoretical aspects of Classical, Semi-Classical and Quantum Molecular Dynamics which are relevant to Chemistry. The topics will therefore include theoretical and computational developments, as well as applications to specific systems in gas phase and condensed media.

Organizer: J.C. Rayez, Laboratoire de Physico-Chimie Moleculaire, Universite Bordeaux - 33405 Talence (F)

Tel: +33 (0)5 56 84 66 08 - Fax: +33 (0)5 56 84 66 45 e-mail: rayez@cribx1.u-bordeaux.fr

Co-organizers: J.A. Beswick IRSAMC Universite Paul Sabatier - 31062 Toulouse (F) Tel: +33 (05) 61 55 60 09 - Fax: +33 (0)5 61 55 60 6 e-mail: beswick@irsamc1.ups-tlse.fr

C. Leforestier LSDSMS - Universite du Languedoc - 34095 Montpellier (F) Tel: +33 (0)4 67 14 33 39 - Fax: +33 (0)4 67 14 48 39 e-mail: lefores@lsd.univ-montp2.fr

Invited speakers having already accepted: F. Aguillon (Orsay), A. Bastida (Murcia), S. Cavalli (Perugia), D. Clary (London), H. Dieter-Meyer (Heidelberg), R. Kosloff (Jerusalem), D. Manolopoulos (Oxford), C. Meier (Toulouse), G. Parlant (Montpellier), O. Roncero (Madrid), R. Schinke (Gottingen), S. Smith (Brisbane), A. Varandas (Coimbra), J.Zhang (New-York).

Students and Postdocs wishing to participate in the meeting and to present a poster may apply for financial aid. The amount of support will depend on our success for attracting external fundings. Please send an abstract as soon as possible to: Philippe Halvick - Laboratoire de Physico-Chimie Moleculaire, Universite Bordeaux, 33405 Talence Cedex (France) Tel: +33 (0)5 56 84 83 77 - Fax: +33 (0)5 56 84 66 45 e-mail: halvick@lpct.u-bordeaux.fr

For more information, check out our web site: http://www.lpcm.u-bordeaux.fr/infos/dynam2000

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

PISA, Italy, June 12-16, 2000

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

The Conference is jointly organised by:

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

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

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

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

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

9. 16TH INTERNATIONAL SYMPOSIUM ON GAS KINETICS

JULY 23rd-27th, 2000 in CAMBRIDGE, U.K.

The 16th International Symposium of Gas Kinetics (gk2k), organised by the Royal Society of Chemistry Gas Kinetics Discussion Group will take place: JULY 23rd-27th, 2000 in CAMBRIDGE, U.K.

The meeting will be held in the Chemistry Department, Cambridge University, and participants will be accommodated in Robinson College, Cambridge.

The scientific programme will include sessions on:

Dynamics and Kinetics of Elementary Reactions

Atmospheric Chemistry

Combustion and Dynamics

Inter- and Intra- Molecular Energy Transfer

Chemistry in Extreme Environments

Plenary Lectures will be given by D.J. Nesbitt, M. Brouard, J.N. Crowley, C.E. Kolb, C.T. Bowman, P.J. Dagdigian, R.E. Miller and P. Andresen. The Polanyi Lecture will be presented by J. Wolfrum and is entitled: "Laser Studies of the Kinetics of Homogeneous and Heterogeneous Processes: From Diatomics to DNA"

We strongly encourage you attend the symposium and to submit abstracts for scientific contributions. To register, please fill in and return the form at:

http://www.gk2k.ch.cam.ac.uk/

either electronically, or to: The Symposium Secretary, 16th International Symposium on Gas Kinetics, University Chemical Laboratory, Lensfield Road, Cambridge, CB2 1EW, U.K. (FAX +44 1223 336362).

Registrations should be returned by:

FRIDAY JANUARY 7TH 2000

A second circular with full details will be sent to all those expressing an interest in Spring 2000.

Further details will be made available on the gk2k website. Other enquiries should be made to the gk2k committee via email to gk2k@atm.ch.cam.ac.uk .

The end of the gas kinetics symposium coincides with twenty-eighth international symposium on combustion, which will take place in Edinburgh, U.K. from 30/7/00 - 4/8/00. Details of that meeting are posted at

http://www.efm.leeds.ac.uk/edin2000/

The gk2k local organising committee. (Dr.R.A. Cox, Dr. D. Husain, Dr. D.M. Rowley and Dr. S.M. Ball)

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@ssci.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/faradischome.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 and SOFTWARE

FREE SOFTWARE RELEASE ANNOUNCEMENT, MultiWell, version 1.01
Macintosh and Unix/Linux versions are currently available. This version includes minor bug fixes and clearly stated copyright information. If you down-loaded the first release (v 1.0), please discard it and download this version in its place. Up-dated versions will be posted periodically.
With minor revisions, the source code can be compiled on other platforms (e.g. Windows). Compressed files can be downloaded from the MultiWell web site.
MultiWell web site: http://aoss.engin.umich.edu/multiwell/
MultiWell calculates time-dependent concentrations, yields, vibrational distributions, and rate constants as functions of temperature and pressure for unimolecular reaction systems which consist of multiple stable species, multiple isomerization reaction channels interconnecting them, and multiple fragmentation channels from each stable species. The stochastic method is used to solve the resulting Master Equation. Users may supply unimolecular reaction rate constants (k(E)’s), sums of states and densities of states (for RRKM theory), or optionally use the Inverse Laplace Transform method. Users can select for weak collision effects different collision models for down-steps including exponential, biexponential, generalized exponential, etc., and user-defined functions. Thermal, chemical activation, or user-defined functions can be used for the initial energy distribution.
The code is intended to be relatively easy to use. It is designed so that very complicated and very simple unimolecular reaction systems can be handled via the data file: no restructuring of the code or recompiling is necessary to handle even the most complex systems.
MultiWell is most suitable for time-dependent non-equilibrium systems. The real time needed for a calculation depends mostly upon the number of collisions during a simulated time period and on the number of stochastic trials needed to achieve the desired precision. For slow reaction rates and precise yields of minor reaction products, the code will require a long run time, but it will produce results. For long calculation runs, we often just let it run overnight.
MultiWell is a new code (1999) based on the Gillespie Exact Stochastic algorithm [1], as developed in our laboratory [2]. It will be described much more fully in a future publication.
For more information, see the MultiWell web site, or contact me.
-John R. Barker jrbarker@umich.edu
[1] (a) D. T. Gillespie, J. Comput. Phys. ,1976, 22, 403; (b) D. T. Gillespie, J. Phys. ,1977, 81, 2340; (c) D. T. Gillespie, J. Comput. Phys. ,1978, 28, 395.
[2] (a) J. R. Barker, Chem. Phys., 77, 201 (1983). (b) J. Shi and J. R. Barker, Int. J. Chem. Kinetics, 22, 187 (1990). (c) J. R. Barker, J. Phys. Chem., 96, 7361 (1992). (d) J. R. Barker and K. D. King, J. Chem. Phys.,

103, 4953 (1995).

Charge and Energy Transfer Dynamics in Molecular Systems

We have the pleasure to announce the first edition of ”Charge and Energy Transfer Dynamics in Molecular Systems” which will be published by Wiley-VCH in December 1999. This book emerged from lectures given to a Physics-Chemistry-Biology audience at different German universities during the last decade. Writing the manuscript it has been our intention to provide a unified introduction into and a common interdisciplinary language for the theoretical treatment of various transfer phenomena in molecular systems. The material spans the range from classical concepts to current areas of research in this field.
For further information please visit our homepage at
http://userpage.chemie.fu-berlin.de/∼manzwww/userpage/kuehn/book.html
Volkhard May (Humboldt University Berlin), Oliver Kuehn (Free University Berlin)

Theory and Application of Quantum Molecular Dynamics

John Z.H. Zhang, 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/