

Molecular Dynamics News

number 98, December 1998

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

The format for MDN is

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 has been accepted - otherwise state *unpublished*).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

MDN is edited by Prof. Vincenzo Aquilanti, Dipartimento di Chimica dell' Università, 06123 Perugia, Italy (electronic mail: AQUILA@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 99 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 (#98). The closing date for issue number 99 is February 1, 1999.

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

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

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

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ANNOUNCING ELECTRONIC DELIVERY OF MDN

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

1. Electronic mail to subscribers

In this case subscribers tell us if they want the newsletter automatically sent to them by electronic mail. The newsletter can be sent in two forms: raw LaTeX source file, or as a Postscript file. Subscribers may specify the desired form.

2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file. A Web browser such as Mosaic or Netscape with suitable viewers allows people to read the files on their computer screens. Alternatively the files can be downloaded for local viewing or printing. Subscribers choosing this delivery option will receive an email announcement when a new issue is posted. For information you are welcome to visit the Molecular Dynamics News World Wide Web site:

<http://www.ucsc.edu/mdn>

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

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

All members of the chemical physics community are invited to join the (free) "molecular-dynamics-news" email list. The "molecular dynamics" in the title is to be interpreted as meaning "dynamical processes in molecules" rather than "classical simulations of molecular motion". The list can be used to distribute details of conferences, vacant academic and postdoctoral positions, changes of address and other news in the Molecular Dynamics field. It also serves as an archive of up-to-date email addresses for people in the field. The list was created by Jeremy Hutson in June 1993 and has now about 1300 members.

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

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

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

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

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review molecular-dynamics-news  
to the address mailbase@mailbase.ac.uk
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Note that messages distributed via the e-mail list are not normally printed in the newsletter, unless the Editors receive an explicit request to do so.

There is also a spectroscopy email list. To join this email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

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join spectroscopy-group John Kennedy
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a. Open Positions

FACULTY

University of East Anglia, Norwich, England

Five new full time academic appointments are to be made in the School of Chemical Sciences at the University of East Anglia, Norwich, England. One of the appointments (number 4 in the list below) is likely to be in the area of Laser chemistry, with particular reference to applications in environmental science. Informal enquiries concerning this post can be made to the author (s.meech@uea.ac.uk) or Prof. David Andrews (d.l.andrews@uea.ac.uk. 01603 592005) Details of the advertisement follow. It is hoped to conduct interviews between the 25 Jan and 5th Feb.

The University has recently announced a substantial investment in the School of Chemical Sciences, enabling it to strengthen core chemistry and to increase its interdisciplinary links with the Schools of Biological and Environmental Sciences, and also with the major science Institutes of the Norwich Research Park.

Accordingly, the School of Chemical Sciences now seeks to build further research strengths in major areas of chemistry, to build further on its successful collaboration with the School of Biological Sciences, and to develop new initiatives with the School of Environmental Sciences. Five faculty posts are available as described below. Whilst it is expected that appointments will be made at lecturer or reader level, depending on the experience and academic record of the applicant, one of the appointments may be made at professorial level for an outstanding candidate. In the case of senior posts, candidates will be expected to provide academic leadership in research, and to further develop links between the School of Chemical Sciences and other UEA Science Schools, members of the Norwich Research Park and national and international research bodies.

Synthetic Organic Chemistry

Researchers with proven expertise in synthetic organic chemistry are welcome to apply. This post would be particularly suitable for those with interests in the synthesis of biomolecular targets such as carbohydrates, nucleic acids and proteins and the development of new synthetic methodology, such as combinatorial chemistry. Applicants seeking to develop collaboration within the Norwich Research Park, especially with the School of Biological Sciences and with microbial and plant scientists in the John Innes Centre, or with food scientists in the Institute of Food Research, will be of particular interest.

Synthetic Inorganic Chemistry

Synthetic inorganic chemists, particularly those relevant to the newly-established Wolfson Laboratory for Environmentally Friendly Catalysis, are invited to apply. The purpose of this Laboratory is to develop and study homogeneous catalysts which avoid the use and production of environmentally harmful substances. Potential catalytic systems of current interest include metal-mediated free radical production, biphasic reactions, biomimetic redox cycling of metal, complexes in aqueous media, metal oxide and hydroxide nanoparticles and reactions in super-critical water.

Biological Chemistry

A protein chemist is sought with interests which will complement existing areas at UEA, such as metalloprotein biology and spectroscopy, and protein structure determination by NMR and X-ray crystallography. The successful candidate will further strengthen the already effective links between the Schools of Biological and Chemical Sciences or be able to exploit the biological strengths within the Norwich Research Park. Research interests in protein structure-function relationships, protein folding, intermolecular interactions or chemical enzymology are particularly welcome.

Physical/Environmental Chemistry

A physical chemist is sought with interests in the application of fundamental theory and/or laboratory techniques relevant to environmental chemistry. Preference may be given to candidates whose research will enhance existing strengths within the School of Chemical Sciences, and help build collaborative research and

teaching programmes with the School of Environmental Sciences. Research strengths in the two Schools relevant to the post include: ultrafast laser spectroscopy, photophysics and photochemical kinetics; condensed phase dynamics; thermodynamics of non-ideal solutions.

Environmental Analytical Chemistry

Applications are invited for a post in Environmental Analytical Chemistry to strengthen research in Analytical Chemistry within the School of Chemical Sciences and to enhance links with the School of Environmental Sciences. The preferred applicant will develop novel measurement strategies and/or techniques for target analyte species of environmental relevance either in the hydrosphere or atmosphere. It is intended that the successful applicant will complement the current research interests of faculty at the Analytical interface in the Schools of Chemical and Environmental Sciences and, as appropriate, across the Norwich Research Park.

Stephen R. Meech, School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, UK e-mail: s.meech@uea.ac.uk, Tele.: 44 (0)1603 593141, Fax: 44 (0)1603 592003

The University of Nottingham

CHAIR IN COMPUTATIONAL and THEORETICAL CHEMISTRY Applications are invited from candidates demonstrating a high level of achievement in computational and/or theoretical chemistry and the leadership to establish a strong computational and theoretical chemistry group at Nottingham. The ability to develop links that underpin research in chemistry and at interdisciplinary interfaces, e.g. with materials engineering, pharmaceutical sciences or biological and medical sciences, will be important. Please quote ref. MCM/085.

Salary for the Chair post will be within the professorial scale, minimum 37,420 pounds per annum.

LECTURER IN COMPUTATIONAL and THEORETICAL CHEMISTRY Applications are invited for a Lectureship in Computational and Theoretical Chemistry. The successful candidate will be expected to develop collaboration with other research areas within the School. Please quote ref. LEG/428.

Salary for the Lecturer post will be within the range 16,655 - 29,048 pounds per annum, depending on qualifications and experience.

Further details and application forms are available from the Personnel Office, Highfield House, The University of Nottingham, University Park, Nottingham, NG7 2RD. Please quote relevant reference number. Fax: 0115 951 5205. Email: Personnel.Applications@Nottingham.ac.uk.

Tel: 0115 951 3260 - Chair posts. Closing date: 15 January 1999. Tel: 0115 951 5927 - Lecturer posts. Closing date: 12 February 1999.

<http://www.nottingham.ac.uk/Personnel/academic.htm#MCM/084&085>, <http://www.nottingham.ac.uk/>, <http://www.nottingham.ac.uk/chemistry/new/>

The University of Manchester,UK, Chair of Physical Chemistry

Applications are invited for this professorial position, which is tenable in the Chemistry Department from 1st October 1999 or earlier, from candidates with outstanding research records in Physical Chemistry.

Applications from candidates with research interests in classical Physical Chemistry will be welcomed, but so will applications from cognate areas of other disciplines; the remit of the Chair will be interpreted flexibly. A Lectureship in Physical Chemistry may be available to support this appointment.

Informal enquiries may be made to Professor Colin Price, Head of Department of Chemistry (tel: 0161 275 4706; fax 0161 275 4273; email Colin.Price@man.ac.uk) or to Professor Gareth Morris (tel: 0161 275 4665; fax 0161 275 4598; email g.a.morris@man.ac.uk).

Application forms (returnable by 21 December 1998) and further particulars are available from the Office of the Director of Personnel, The University of Manchester, Manchester M13 9PL; tel: ++44 (0) 161 275 2028; fax: ++44 (0) 161 275 2221; email: personnel@man.ac.uk; web site <http://www.man.ac.uk>. Please quote the reference no. 828/98. As an equal opportunities employer, the University of Manchester welcomes

applications from suitably qualified people from all sections of the community regardless of race, religion, gender or disability.

University of Utah

A full time Research Associate position is available in the DOE Accelerated Strategic Computing Initiative (ASCI) Center at the University of Utah. Salary will be \$60K per year with full benefits. The applicant must have a doctoral degree in a scientific discipline, in addition to experience in object oriented programming, including the use of C++, and experience with a Unix OS (SGI preferred) and scientific programming. Experience with FORTRAN programming, MPI parallelization, molecular dynamics, and/or electronic structure codes is desirable. The applicant must have the ability and desire to work in a high profile interdisciplinary environment.

A vitae, publication list, and three letters of recommendation should be sent to: Professor Gregory A. Voth, Director, Henry Eyring Center for Theoretical Chemistry, Department of Chemistry, University of Utah, 315 S. 1400 E. RM Dock, Salt Lake City, Utah 84112-0850, voth@chemistry.chem.utah.edu, (801) 581-4353 (fax), Web Site: <http://voth.chem.utah.edu/>

Howard University

Two or more positions at the Assistant Professor level are open in PHYSICAL and ANALYTICAL chemistry. Targeted areas include separations, surface, polymer, atmospheric and laser chemistry. Applications should include a resume and a brief statement of proposed research. Send application and three letters of recommendation to Search Committee, Department of Chemistry, Howard University, Washington, DC 20059. Evaluation of applications will begin December 15, 1998 and continue until suitable candidates have been found. Outstanding applications in other areas will be considered. For further information about the department, see: <http://www.chem.howard.edu>

FACULTY POSITION IN EXPERIMENTAL PHYSICS The University of Chicago

The Department of Physics, the Enrico Fermi Institute, and the James Franck Institute of the University of Chicago expect to have a faculty position in experimental physics available at the Assistant Professor level, beginning in autumn 1999. We are especially interested in candidates with outstanding research accomplishments in the areas of atomic physics, optical trapping and cooling, biophysics, or structural studies of condensed matter. Candidates must have demonstrated a high degree of excellence in research, and must have a strong interest and ability in teaching.

Completed applications received by October 30, 1998, will be given full consideration. Applicants should send a resume, list of publications, and a description of their research to the address below, and should arrange for three letters of recommendation to be sent directly to the same address: Prof. Frank Merritt, Chairman; Department of Physics; Experimental Physics Search; The University of Chicago, 5720 S. Ellis Ave., Chicago, IL 60637-1434. The University of Chicago is an equal opportunity/affirmative action employer. <http://ars-www.uchicago.edu/physics/>

POST DOCTORAL AND VISITING

POSTDOCTORAL POSITION, National Tsing Hua University, Taiwan

Two postdoctoral positions starting 1999 (flexible) at the Department of Chemistry, National Tsing Hua University, TAIWAN. Possible projects include: (1) Two-color resonant four-wave mixing spectroscopy of free radicals in a supersonic jet, (2) Time-resolved Fourier-transform Spectroscopy with a step-scan FTIR - spectroscopy, kinetics, and dynamics after laser photolysis of gaseous molecules. (3) Photoionization spectroscopy and kinetic of free radicals using synchrotron radiation source or VUV laser. (4) Ultrafast phenomena - photodissociation and charge transfer mechanisms. Extended experiences with excimer and

Nd-YAG lasers preferred. Good salary with yearly renewable appointment. Applicants should arrange 2-3 letters of recommendation to be sent to Prof. Y. P. Lee, I-C. Chen, Department of Chemistry, National Tsing Hua University, TAIWAN 300 (e-mail: yplee@net.nthu.edu.tw, icchen@net.nthu.edu.tw, FAX: 886-3-5722892)

POSTDOCTORAL POSITIONS, ETH, Zuerich

Two postdoctoral positions are open in the molecular kinetics and spectroscopy group of Martin Quack at ETH Zuerich for two new projects. The first project involves investigation of intramolecular primary processes on short (fs to ps) timescales (IVR and simple reactive processes such as stereomutation). In this project it is planned to study the same type of process by two techniques in parallel. 1. High resolution spectroscopy and fully time dependent quantum dynamics derived from this and 2. Femtosecond time resolved techniques. Whereas the first approach has been developed by our group over many years and the know how is available, new experiments are being built during for fs to ps time resolved spectroscopy. It would be useful for applicants to have experience with fs laser techniques.

The second project is situated in the framework of the alliance for global sustainability (AGS) and involves development of new high resolution (FTIR and laser) spectroscopic techniques for atmospheric spectroscopy. Applicants should be enthusiastic about these applications of spectroscopy, they should have adequate familiarity with high resolution spectroscopy, and should be willing to collaborate in an international framework. Both positions are available immediately for one year, renewable for one or more years upon mutual agreement. The salary is Sfr 60000.- per year (about 40000 USD). The positions would also be available to particularly gifted graduate students (the salary is then about 60 percent of the above amounts). Send applications to Prof. Martin Quack, Lab. for Physical Chemistry, ETH Zuerich (Zentrum), CH-8092 Zuerich, Switzerland.

Postdoctoral Positions, University of California, Berkeley

Two postdoctoral positions are available in the research group of Daniel Neumark at UC Berkeley. One position is in the field of molecular beam reaction dynamics. Research will focus on photodissociation and reactive scattering of hydrocarbon radicals using molecular beam instruments in my laboratory and at the Advanced Light Source. The second position is in the area of negative ion photoelectron spectroscopy. Research will be centered on studies of size-selected clusters, radicals, and transition states. A strong background in experimental chemical physics is required for both positions. Applicants should send their CV, publication list, and names of three references to: Professor Daniel Neumark, Department of Chemistry, University of California, Berkeley, CA 94720, USA

POSTDOCTORAL RESEARCH ASSOCIATE, University of North Carolina at Chapel Hill

Applications are invited for a one to two-year postdoctoral research position funded under the EPA STAR Grant project "Aerosol Partitioning and Heterogeneous Chemistry," in the research group of Dr. Roger Miller. The group's research focuses on investigating the chemical and physical properties of tropospheric and stratospheric aerosols.

The successful candidate will be involved in the development and implementation of an in situ spectroscopic technique for monitoring the composition and heterogeneous chemistry of tropospheric aerosols. This technique involves the combination of step-scan FTIR spectroscopy, tunable diode laser spectroscopy and laser induced thermal desorption. The aerosols of interest include those currently being considered by the EPA as a component in future PM_{2.5} regulations. The goal is to develop non-invasive in situ methods for determining the properties of these semivolatile species.

Candidates are expected to have a PhD in chemistry, atmospheric science or related field. Experience with spectroscopy and lasers is necessary. Please send CV, a letter describing research interests and background, relevant publications and at least two letters of reference to Professor Roger E. Miller, Department of Chemistry, CB3290, Kenan Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC

27599-3290, USA. Phone 919-962-0528, fax 919-962-2388, remiller@unc.edu.

POSTDOCTORAL POSITION, UNIVERSITY OF BORDEAUX, FRANCE

A postdoctoral position (12 months) is available at the "Laboratoire de Physico-Chimie Moleculaire" of the "Universite Bordeaux I", France. The position is funded by the European Commission under the TMR network "Astrophysical Chemistry" program. The network involves eight research groups : Ian Smith and Ian Sims (University of Birmingham, GB), David Clary and David Williams (U.C. London, GB), Jurgen Troe (University of Goettingen, DE), Dieter Gerlich (University of Chemnitz, DE), Piergiorgio Casavecchia (University of Perugia, IT), Bertrand Rowe (University of Rennes, FR), Evelyne Roueff (Observatory of Paris, FR), Michel Costes and Jean-Claude Rayez (University of Bordeaux, FR). The focus at Bordeaux is on experimental and theoretical studies of exoergic bimolecular reactions that might be important in the chemistry of interstellar clouds. 1. Experimental project. Experiments are conducted on a recently developed crossed-molecular beam apparatus, which allows for scanning the relative translational energy of reactants down to values (4 meV) relevant to the conditions of the interstellar medium. Reactions of C or Si atoms with O₂ and unsaturated hydrocarbons are investigated. Detection of reactants and products is by laser-induced fluorescence in the visible, ultra-violet or vacuum ultra-violet. 2. Theoretical project. Efforts are focused on the determination of the potential energy surfaces involved in neutral-neutral or ion-neutral three-atom reactions like C + CH, (C⁺) + CH, C + (CH⁺), ... in order to estimate the rate constants of different open channels and the branching ratios. Dynamical aspects of some of these reactions could also be investigated. Important ! Only applications from nationals of the European Union (France excluded) or Associate States (Iceland, Israel, Liechtenstein and Norway) can be received. Net salary will be around 12000 FF/month. In addition, the postdoc associate will have funds to spend up to one month in another laboratory of the network. Candidates (with a PhD in chemistry or physics or who expect to obtain the diploma in the following months) interested by one of these projects should submit a CV and the names of one or two referees to:

Dr Michel Costes, UMR 5803 CNRS - Universite Bordeaux I, Laboratoire de Physico-Chimie Moleculaire, Universite Bordeaux I, 33405 Talence Cedex, France, phone: 33 5 56 84 63 45, fax: 33 5 56 84 66 45, email: costes@cribx1.u-bordeaux.fr

POSTDOCTORAL APPOINTMENT, UNIVERSITY of OXFORD, UK

Applications are invited for a postdoctoral position in the Physical and Theoretical Chemistry Laboratory to work with M.S. Child on ab initio Rydberg dynamics. The aim is to combine an ab initio R matrix treatment of the electrons with the multichannel quantum defect approach to the nuclear motions, with a view to modelling ionization, dissociation and dissociative recombination processes. Knowledge of ab initio quantum chemistry and/or multichannel quantum defect theory is highly desirable. The tenure of the appointment is for up to two years on a salary scale between 17570 and 20107 GBP pa, according to age and experience. Applications including a cv and contact details for two academic referees should be sent to Prof M.S. Child, Physical and Theoretical Chemistry Laboratory, South Parks Rd, Oxford OX1 3QZ, UK. Fax +44 1865 275410 (see <http://physchem.ox.ac.uk/msc/> for further details)

POST-DOCTORAL POSITIONS, University of California, Berkeley

Opportunities are available on the new Chemical Dynamics Beamline at the Advanced Light Source to study reaction dynamics and photochemistry of radicals and clusters. This unique User Facility (<http://www.lbl.gov/chemicaldynamics>) features a 10cm undulator providing 1e16 VUV photons/second continuously tunable from 5 to 30 eV, along with dedicated molecular beam endstations using both neutral time-of-flight as well as ion imaging detection methods in addition to extensive laser resources. Successful candidates will be expected to develop new radical and cluster molecular beam sources; perform studies of radical photochemistry, crossed-beam reaction dynamics or cluster spectroscopy and dynamics; develop innovative applications of synchrotron radiation to chemical dynamics studies such as coincidence

imaging studies of neutral photochemistry; perform collaborative studies with outside users; publish results in recognized journals.

These positions require a PhD in Chemical Physics or a related discipline, experience in molecular beam photochemistry or reaction dynamics studies and a record of publication in chemical dynamics or a closely related field. Experience with synchrotron radiation is useful but not necessary.

Interested applicants should send a CV and arrange for two letters of recommendation (email preferred) to: Dr. Arthur G. Suits, Chemical Dynamics Group, MS 6-2100, 1 Cyclotron Road, E. O. Lawrence Berkeley National Laboratory, Berkeley CA 94720 USA, Tel +1 510-486-4754, Fax +1 510-486-5664, Internet agsuits@lbl.gov, <http://www.lbl.gov/~agsuits>

POSTDOCTORAL POSITION, Naval Research Laboratory, Washington, D.C.

Postdoctoral research positions in experimental physical chemistry are available for qualified candidates in the Chemistry Division at the Naval Research Laboratory, Washington, D.C. The opportunity is for femtosecond laser studies of molecular dynamics, such as energy transfer and photodissociation. Projects include studies of molecules in gases, liquids and on interfaces. Applicants familiar with ultrafast lasers and molecular dynamics are preferred. Fellowships are awarded through the NRC, and appointments are for a minimum of one year, renewable to two years. The annual stipend is \$48,000. Information on our research, including a publication list, and links to the NRC Postdoctoral Program can be found on our webpage, <http://chem1.nrl.navy.mil/molecular>

For more information, please contact: Jeff Owrutsky, Code 6111, Naval Research Laboratory, Washington, D.C. 20375-5342, (202)-404-6352 [voice], jeff@chem1.nrl.navy.mil (U.S. Citizens only.)

Postdoctoral Research Position in Surface Probe Microscopy

Our group is interested in chemical and physical processes at solid/liquid interfaces. The laboratory is well equipped with STM/AFM, in addition to nsec, psec, and fsec lasers for linear and nonlinear optical laser experiments. Our work is supported by NSF, DOE, and Research Corporation.

The objective of the current project is to study interface dynamics and will ultimately involve combining SPM and optical probes. This is a good opportunity for an individual with strong SPM skills seeking to learn more about optical probes of interfaces. Candidates should have previous experience with STM/AFM. Experience with lasers is a plus. The candidate should have strong problem solving skills, work well with others and demonstrate scientific leadership and initiative.

The Surface Science Center at the University of Pittsburgh provides an excellent research environment. The city of Pittsburgh is safe, pleasant and affordable.

The position is for one year, with possibility of renewal. Applicants should submit a curriculum vitae, a list of publications, a reprint of their most significant work, a statement of research interests and objectives, as well as names and addresses of three references who are willing to write letters of recommendation.

Dr. Eric BORGUET, Department of Chemistry and Surface Science Center, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh PA 15260, (412) 624-8304 Office, (412) 624-8305 Lab, (412) 624-8611 Fax, borguet+@pitt.edu, <http://www.chem.pitt.edu/faculty/borguet.html>

POSTDOCTORAL POSITION, VRIJE UNIVERSITEIT, AMSTERDAM

In the ACAS (Analytical Chemistry and Applied Spectroscopy) department of the Chemistry Division, Faculty of Sciences, a two-year postdoctoral position is available in laser spectroscopy. In this department a new line of experimental physical-chemistry research is initiated in the field of dynamic processes in the condensed phase, using an advanced lasersystem, in a newly built laserlab. The aim of this research is to obtain insight in excitation transport and excitation relaxation in complex systems, such as porphyrin clusters and films, and porphyrin-protein complexes. The successful candidate will be expected to perform time-resolved resonance Raman and fluorescence spectroscopy on condensed phase systems, on a pico to nanosecond time scale, as part of the program "Spectroscopy and Dynamics of Complex Systems", and to

(co)-supervise graduate and undergraduate students in this project. A contribution to the teaching activities of ACAS is also expected. Applicants should have a PhD in physical chemistry, and have practical experience in the field of time resolved laser spectroscopy. Demonstrated interest in (bio)-physical systems would be an advantage.

Further information may be obtained from Prof. Dr. C. Gooijer, (31-20-4447540) or Dr. G. van der Zwan (31-20-4447635, zwan@chem.vu.nl, FAX: 31-20-7643). Applications, including a curriculum vitae, should be addressed to Drs. G. Veerbeek, Faculty of Sciences, de Boelelaan 1081 a, 1081 HV, Amsterdam.

POSTDOCTORAL POSITION, UNIVERSITY COLLEGE, LONDON

A three-year EPSRC funded Postdoctoral Research Assistantship in Theoretical Molecular Physics is available. 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 £ 15,735 –£ 22,785 p.a. plus £ 2134 London weighting.

Further information can be obtained from: Jonathan Tennyson, Department of Physics and 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, Michigan State University

A postdoctoral position is available in the general area of Femtosecond observation and control of chemical reactions in the research group of Marcos Dantus.

Because funding for this position will come from an Affirmative Action Postdoctoral Fellowship from the College of Natural Science at MSU candidates for the fellowship must be Black, Hispanic, Asian/Pacific Islander or Native American and must be U.S. Citizens or U.S. permanent residents.

This position includes a generous stipend and health coverage.

For information about our research group and about other opportunities visit our web page at: www.cem.msu.edu/~dantus

For further information or to apply (C.V., and two letters of recommendation required) contact Professor Dantus directly at dantus@cem.msu.edu

Postdoctoral Position, Stanford University

A postdoctoral position is available in my research group at Stanford University in the area of semiconductor surface chemistry and semiconductor processing. The research will focus on in situ optical spectroscopic studies of chemical vapor deposition, chemical etching, and surface modification of group IV semiconductors. Techniques such as MIR-FTIR spectroscopy and REMPI are combined with mass spectrometry, scanning probe microscopy, and surface analytical techniques to investigate the reaction mechanisms, kinetics, and dynamics of these processes at the molecular level.

An enthusiastic, hardworking individual with a strong background in laser spectroscopy and/or surface science is preferred. The initial appointment will be for one year, with the option of a second year upon mutual agreement. The position is available immediately, but later dates may be arranged.

Applicants should submit a resume and have two letters of recommendation sent to Prof. Stacey Bent, Department of Chemical Engineering, 381 North-South Mall, Stanford University, Stanford, CA 94305-5025, or e-mail: stacey.bent@stanford.edu.

Stanford University is an equal opportunity / affirmative action employer encouraging applications from women and minority candidates.

Postdoctoral Position, University of Utah

A postdoctoral position is available immediately in the lab of Scott Anderson at the University of Utah. The experiment combines a flow tube reactor with a tandem guided ion beam mass spectrometer to study the unimolecular decomposition mechanisms of strained high-energy-density molecules (e.g. cubanes, quadricyclanes, bicyclobutanes). Ab initio calculations are carried out to aid interpretation. A secondary goal of the experiments is to test applications of low energy guided ion beam scattering to analytical mass spectrometry, and resolution of strained and chiral isomers will be investigated. More information on the instrument can be found in Int. J. Mass Spectrom. Ion Proc. 167/168 (1997) 269, or at the following web address: www.chem.utah.edu/chemistry/faculty/anderson/anderson.html. More information can be found in preprints, available upon request.

Experience with ion beams or mass spectrometry is helpful, however, the most important criterion is creativity. The initial appointment will be for one year, and is renewable for a second year based on progress and availability of funds. 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 is encouraged. If interested, please send a CV and arrange for three letters of recommendation to be sent to: Prof. Scott L. Anderson, Chemistry Dept., University of Utah, 315 S. 1400 E., Salt Lake City, UT 84112.

Prof. Scott L. Anderson, Chemistry Department, University of Utah, 315 S. 1400 E. RM Dock, Salt Lake City, UT 84112-0850, Ph:(801)585-7289, FAX:(801)581-8433, anderson@chemistry.utah.edu, <http://www.chem.utah.edu/chemistry/faculty/anderson/anderson.html>

POST-DOCTORAL AND RESEARCH FACULTY, University of California, San Diego

The Kent Wilson group, at the University of California, San Diego, Dept. of Chemistry and Biochemistry, has positions available for exceptionally talented experimental scientists in the following areas: ultrafast x-ray diffraction and absorption applied to chemical and biochemical dynamics and function, and new techniques in optical microscopy for spatially and temporally resolved imaging as applied to the understanding of dynamics of cellular and intercellular biomolecular and biological processes (including interneuronal communication and function). For more information about these positions and the group, or to receive application process information, visit our Web site, <http://www-wilson.ucsd.edu> OR email wgjobops@ucsd.edu. Positions commensurate with experience and qualifications, with salaries based on UC pay scales.

POSTDOCTORAL POSITION, NAVAL RESEARCH LABORATORY

I am looking for a postdoctoral candidate in the Chemistry Division at the Naval Research Laboratory. These positions are administered by the National Research Council (NRC) and attract a nationwide pool of applicants. The candidate will work in a new research area measuring the fast kinetics of protein folding and conformational changes in synthetic biomaterials. I also intend to expand the program to low temperature measurements and begin to produce proteins and mutants of interest by recombinant DNA methods. The candidate's background should include at least two of the four areas: laser experience, infrared spectroscopy, a kinetics background, and knowledge of biological materials or systems. The instrumentation available in my laboratory includes: a Nd:YAG pulsed laser, a vacuum step-scan FTIR, a Raman shifter, a temperature programmed cell, a separate cold finger and chamber for low temperature experiments, and basic microbiology equipment. Other equipment for protein characterization, such as a CD spectrometer, UV spectrometers, and differential scanning calorimetry are available on site. This research opportunity and postdoctoral research program is described on the world wide web at <http://dynamics-www.nrl.navy.mil/molecular/> and my web site is: <http://dynamics-www.nrl.navy.mil/molecular/jane/jane.html>.

The postdoctoral candidates at the Naval Research Laboratory must be U.S. citizens. Initial appointments are for one year and are routinely renewable for a second year. The stipend is \$47,000 per year with additional funds for moving expenses and professional travel to meetings.

The applicant is responsible for selecting a research project and writing a short research proposal in collaboration with the prospective advisor. It is my experience that the application proposal takes about four weeks to complete. The deadlines for applications are 15 January 1999 and 15 April 1999, with the earliest possible starting times of July 1999 and October 1999, respectively. For further information please contact me through e-mail or by phone. Please post or share the attached announcement with your colleagues.

Dr. Jane K. Rice, Chemistry Division, Code 6111, Phone 202 767-0721, FAX 202 404 -8119,
Rice@ccf.nrl.navy.mil

POSTDOCTORAL POSITION, TEXAS TECH UNIVERSITY

I have a post-doctoral position available January 1, 1999, in my lab at Texas Texas Tech University. The research involves photoelectron spectroscopy of metal hydride anions, such as LiH_2^- , MgH_3^- , BH_4^- , and AlH_4^- . The desired candidate would have experience in laser spectroscopy, electronics, and computer programming. Experience with vacuum systems and mass spectrometry would also be helpful, but not required.

Applications, including a CV and 2 letters of recommendation, should be sent to:

Prof. Paul G. Wenthold, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409-1061, Ph (806) 742-3088, FAX (806) 742-1289, email: wenthold@dorothy.chem.ttu.edu
Texas Tech is an EE/AA employer.

POSTDOCTORAL POSITION, ARGONNE NATIONAL LABORATORY

A post-doctoral position is available in the Chemical Dynamics Group at Argonne National Laboratory. The research involves development and application of laser based experimental methods in high-temperature gas-phase kinetics in the laboratory of Jan P. Hessler. The successful candidate will be expected to measure the rates of reactions under non equilibrium conditions, perform state-to-state relaxation measurements, and study important dissociative and associative reactions. The results obtained from these experiments will be analyzed with state-of-the-art Master Equation and Monte Carlo techniques. The Chemistry Division of Argonne National Laboratory has a strong Chemical Dynamics Group, composed of several theoretical chemists and experimentalists, and the successful candidate will be encouraged to interact with others in the group and to develop new research ideas. The position is available immediately. However, depending upon circumstances, the successful candidate may choose to start in the coming Spring or Summer. Please send a curriculum vitae and have two letters of recommendation sent directly to Dr. Jan P. Hessler, Chemistry Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439-4831, Communication via electronic mail or facsimile to 1-630-252-4470 are acceptable.

POSTDOCTORAL POSITION, National Research Council of Canada

A postdoctoral position in theoretical chemical physics is available. The successful candidate will choose one (or more) of several planned research projects in the general fields of: (1) Molecular dynamics in intense and/or short-pulse laser fields (2) Reaction dynamics at interfaces (3) Mathematical method development.

The starting date is flexible.

For more information about recent and ongoing research projects see

<http://gold.nrc.ca/~tamar>

For any other information please contact me at tamar@mahler.sims.nrc.ca or at Tel. 613-990-0945.

e-mail: tamar.seideman@nrc.ca, <http://gold.nrc.ca/~tamar>

Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Drive, Ottawa, Ontario K1A 0R6, Phone: (613) 990-0945, FAX : (613) 947-2838

POSTDOCTORAL POSITION, New York University

A postdoctoral position is available immediately in the group of Prof. John Z.H. Zhang at New York University. The prospective candidate should have a good background in theoretical chemistry with good programming skills. The area of research is somewhat flexible depending on the candidate's background and strength. If any person is interested, please send me a short cover letter with a cv and two letters of recommendation to me at the following address.

New York city provides a unique and exciting environment for any person who is interested in big city living. John Z.H. Zhang Professor of Chemistry Department of Chemistry New York University New York, NY 10003 Tel. 212-998-8412 Fax. 212-260-7905 zhang@risc.nyu.edu zhang@p150.chem.nyu.edu <http://risc.nyu.edu>

POSTDOCTORAL ASSOCIATE, Ohio State University

We are beginning a new set of experiments that resolve the directions of both the velocity and angular momentum vectors of products produced in crossed molecular beams, and the new postdoc will be heavily involved in that project. Experience with pulsed molecular beams, lasers, and imaging hardware are all useful, but talented candidates from quite different backgrounds will be considered. Opportunities also exist for collaboration with the Chemical Dynamics Imaging group at Sandia National Laboratory.

Information on our interests and several reprints and preprints are available at <http://www.chemistry.ohio-state.edu/~mcbane/research.html>

The position is open for one year with a second year possible depending on mutual satisfaction and available money. To apply, send a CV and arrange for two or three letters of recommendation to be sent to the addresses listed below.

George McBane, Department of Chemistry, Ohio State University, 100 W. 18th Ave, Columbus, OH 43210, mcbane.2@osu.edu, phone (614) 292-4098, fax (614) 292-1685

POSTDOCTORAL APPOINTMENT, Argonne National Laboratory

The Gas Phase Chemical Dynamics Program at Argonne National Laboratory has an opening for a postdoctoral appointment working with R. Glen Macdonald. The research involves the use of high resolution time-resolved near infrared and infrared absorption spectroscopy to study the spectroscopy, dynamics and kinetics of radicals of interest to combustion and atmospheric chemistry. The main thrust of the program over the next few years will be to study the dynamics and kinetics of atom + radical and radical + radical processes; however, other studies are possible, depending on the qualifications and interests of the successful candidate. Several recent articles will give potential candidates an idea of the variety of problems that can be tackled with this apparatus; a) Infrared Spectroscopy, *J. Mol. Spectroscopy* 186, 349 (1997). b) Chemical Kinetics, *J. Phys. Chem.* 102, 4585 (1998), and c) Chemical Dynamics, *J. Chem. Phys.* 109, Sept. 15 (1998). The successful candidate should be planning to graduate soon or be a recent graduate from a Chemical Dynamics or Kinetics Program, and have experience in laser spectroscopy, vacuum techniques, and computer data acquisition. A background in rovibrational spectroscopy of polyatomic molecules would be a desirable asset. An application will require a CV and three letters of recommendation. For further information, interested candidates should contact Glen Macdonald.

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

R. Glen Macdonald Ph. (630) 252-7742 Argonne National Laboratory Fax. (630) 252-4470 Chemistry Division Email. macdonald@anlchm.chm.anl.gov 9700 South Cass Ave. Argonne, IL 60439

POSTDOCTORAL POSITIONS, Korea Advanced Institute of Science and Technology

Two postdoctoral positions are available to study high resolution spectroscopy and photodissociation dynamics of alkali metal clusters in molecular beam. The focus will be on the selective control of photodissociation of alkali dimers or trimers. The applicant should have knowledge on nanosecond dye laser and/or molecular beam. The contract is one or two years. Salary is around 20,000 dollars per year and negotiable. We have developed new high temperature supersonic jet generator. We are one of the Creative Research Initiative Center in Korea and have good laser and molecular beam facility with sufficient research funding to build and buy new machines. Interested candidates should send e-mail to Prof. Bongsoo Kim at "bongsoo@kaist.ac.kr" or call 82-42-869-2836 (fax)82-42-869-2810

POSTDOCTORAL POSITION, CHEMICAL DYNAMICS GROUP, EXTRATERRESTRIAL CHEMISTRY, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA, TAIWAN, ROC

A post doctoral position is open in the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, ROC. The primary mission of the candidate is to investigate chemical dynamics of CN and C₂H reactions with unsaturated hydrocarbons relevant to the chemistry in the atmosphere of Saturn's moon Titan employing crossed molecular beams experiments. The results of these investigations are expected to play a significant role to understand data of the Cassini probe - a Saturn bound spacecraft analyzing Titan's atmosphere. Pertinacious energetic candidates should send inquiries to Dr. Ralf I. Kaiser, Institute of Atomic and Molecular Sciences, Academia Sinica, 1 Section 4, Roosevelt Rd., Taipei, 106, Taiwan, ROC. Tel:886-2-23645370; Fax:886-2-23620200; email:kaiser@po.iams.sinica.edu.tw. <http://po.iams.sinica.edu.tw/~kaiser>.

POSTDOCTORAL RESEARCH ASSOCIATE IN PHYSICAL CHEMISTRY, University of Bern, Switzerland

A new postdoctoral position is available in the division of Space Research and Planetary Sciences at the Physikalisches Institut (Institute for Experimental Physics) of the University of Bern, Switzerland. The successful applicant is expected to be a recent PhD recipient and have demonstrated expertise in neutral and ion chemical gas dynamics, and/or heterogeneous reactions with water and acids in different phases using techniques such as mass spectrometry, high resolution spectroscopy, flash laser photolysis, etc. He/she will work in collaboration with members of our institute on the construction and calibration of the experiment ROSINA onboard ESA's space mission Rosetta to comet Wirtanen as well as conduct independent laboratory research relevant to the physics and chemistry of comets, asteroids and planetary atmospheres. Interested candidates should send a CV summarizing their research interest and experience, a list of publication, names and address (preferable e-mails) of three professional references by November 30, 1998 to: Prof. E. Kopp, Physikalisches Institut, University of Bern, Sidlerstrasse 5, CH-3012 Bern, Switzerland. E-mail: ernest.kopp@phim.unibe.ch

POSTDOC POSITION FOR TWO YEARS: Do Rydberg atoms go commercial?

The group of Bart Noordam at the FOM-Institute for Atomic and Molecular Physics in Amsterdam, Netherlands, will start a project in which we explore the possibility to construct an ULTRAFAST INFRARED IMAGING CAMERA.

The aim of this project is to design and construct a prototype of an imaging camera that operates throughout the infrared part of the electromagnetic spectrum: $\lambda = 1 \text{ micron} - 1 \text{ mm}$. The photo-sensitive film is based on gas-phase Rydberg atoms (patented). A unique feature of the camera is the combination of infrared sensitivity and ultrashort exposure times (as low as 1 ns). The project is a challenging combination of applied and fundamental physics.

We are seeking a candidate who I) is interested in developing a new type of instrument (see e.g. ref. [1]) and II) is interested in doing fundamental research (far-infrared photoionization properties of Rydberg atoms see e.g. ref. [2,3]). For further information see: www.amolf.nl/external/positions/noordam/ultrafast.html or

email to noordam@amolf.nl

[1] A streak camera operating in the mid-infrared M. Drabbels, and L. D. Noordam Optics Lett. 22, 1436 (1997) [2] Far infrared four-photon ionization of lithium Rydberg atoms bypassing a Cooper minimum J. H. Hoogenraad, R. B. Vrijen, P. W. van Amersfoort, A. F. G. van der Meer, and L. D. Noordam Phys. Rev. Lett. 75, 4579 (1995) [3] Decay of oriented Rydberg wavepackets excited with far-infrared radiation G. M. Lankhuijzen, M. Drabbels, F. Robicheaux, and L. D. Noordam Phys. Rev. A 57, 440 (1998)
L. D. Noordam, FOM-Institute for Atomic and Molecular Physics Kruislaan 407, 1098 SJ Amsterdam, The Netherlands, Tel.: (31) 20 - 608 1354 (direct), Fax.: (31) 20 - 668 4106
homepage: www.amolf.nl/external/wwwlab/atoms/femtophys

POSTDOCTORAL POSITION, UNIVERSITY of MONTREAL

A postdoctoral position is available in the group of Tucker Carrington Jr. at the University of Montreal, Canada The initial appointment will be for one year but funds are available for a second year. Candidates should have training in either theoretical chemistry or theoretical physics. Experience in quantum dynamics calculations would be an asset.

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

Interested candidates should send a C.V. and a summary of research interests to Professor Tucker Carrington Jr., Departement de chimie, Universite de Montreal, Case postale 6128, succursale Centre-ville, Montreal (Quebec) H3C 3J7, Canada
tel: (514) 343-2123, fax: (514) 343-7586, e-mail: Tucker.Carrington@umontreal.ca

POSTDOCTORAL POSITIONS IN MOLECULAR LASER SPECTROSCOPY AND CHEMICAL KINETICS

(NOTE: INDIVIDUALS WHO RESPONDED TO AN EARLIER AD NEED NOT REAPPLY BECAUSE THEIR APPLICATIONS ARE ON FILE)

Two postdoctoral research associate positions will be available in October/November in molecular laser spectroscopy and chemical kinetics at Mississippi State University's Diagnostic Instrumentation and Analysis Laboratory (DIAL). DIAL is a multidisciplinary research and development institute, funded predominantly by the Department of Energy and the National Aeronautics and Space Administration. The major emphasis of our research programs concerns application of modern instrumentation, including lasers, to environmental, combustion and propulsion problems. Many of the projects have both basic and applied aspects. The research associate for the first project will work on application of laser spectroscopy (especially cavity ring-down spectroscopy, photoionization/time-of-flight mass-spectrometry, and laser-induced fluorescence) to environmental/combustion problems. This position will start in ~October/November. He/she should have a strong background in laser spectroscopy or a related area. The associate for the second project will work on the kinetics of metal oxide formation, especially at high temperatures. He/she should have experience in kinetics, preferably with flow reactors. Familiarity with use of lasers and mass spectrometers for species detection will be an asset. This position starts in ~November.

The associates can expect a salary of \$30-32K per year, plus medical insurance and moving expenses.

Interested individuals with appropriate research background should promptly send a cover letter and a cv (preferably by e-mail or fax) and have 2-3 recommendation letters sent directly to: Dr. R.Vasudev, Mississippi State University, Diagnostic Instrumentation and Analysis Laboratory, 205 Research Boulevard, Research and Technology Park, Starkville, MS 39759-9734; Fax:(601)-325-8465; E-mail: vasudev@dial.msstate.edu. Evaluation of applications will begin in September/October. We are an equal

opportunity, affirmative action institution.

Ram Vasudev, Mississippi State University, Diagnostic Instrumentation and Analysis Laboratory, 205 Research Boulevard, Starkville, MS 39759-9734

Phone: (601)-325-0499 (Office); (601)-325-9039 (Lab); Fax: (601)-325-8465; E-mail:

vasudev@dial.msstate.edu

POSTDOCTORAL POSITION, Hanscom Air Force Base A postdoctoral position for work in theoretical chemical dynamics is available at the Air Force Research Laboratory, Hanscom Air Force Base (about 10 miles north of Boston), MA. Successful candidates are expected to calculate cross sections for inelastic and reactive involving atom-molecule or molecule-molecule collisions. Position initially for one year - with a possibility for renewal for another year. Commensurate salary. U.S. citizenship or Green Card required. Reply to: sharma@plh.af.mil.

POSTDOCTORAL POSITION, HEBREW UNIVERSITY OF JERUSALEM

A Post-doctoral position in the field of "electronic structure theory of large systems" is available in the group of Dr. Roi Baer at the Dept. of Physical Chemistry, the Hebrew University, Jerusalem Israel.

The research focuses on developing novel theoretical models and numerical methods to study the properties of very large atomic and molecular systems. Specifically, much research will be devoted to developing linear scaling methods for electronic structure and will include the incorporation of the new ideas and techniques into a fast Kohn-Sham DFT code.

Recent developments we have made can be found in: <http://chem.ch.huji.ac.il/employee/baerr/ibaerr.htm>.

Starting date is flexible -end of this year or beginning of next. Please send curriculum vitae and the names of three references to: Dr. Roi Baer, Dept. of Physical Chemistry, Hebrew University, Jerusalem 91904, Israel or via email to roib@fh.huji.ac.il.

POSTDOCTORAL POSITION IN ATMOSPHERIC PHYSICAL CHEMISTRY

Candidates are sought for a postdoctoral position at the University of Chicago in the field of atmospheric physical chemistry. Funded by a prestigious award from the Camille and Henry Dreyfus Foundation, this position provides an opportunity for outstanding chemists to perform research in environmental science. The salary set by the Dreyfus Foundation is \$35,000/yr. The visiting scientist will work in the laboratories of Prof's. L. Butler and/or J. Abbatt, in a program designed jointly with the visiting scientist to maximize his/her ease of entree into this interdisciplinary area. Potential projects include: photochemistry of atmospheric species, the optical properties of aerosols, and atmospheric heterogeneous chemistry.

Candidates should send a cv, letter of research interests, and the names and addresses of three potential references to either Prof. L. J. Butler, James Franck Institute and Dept. of Chemistry, The University of Chicago, 5640 S. Ellis Ave., Chicago, IL, 60637 or Prof. J. Abbatt, Dept. of the Geophysical Sciences, The University of Chicago, 5734 S. Ellis Ave., Chicago, IL, 60637, by Sept. 30, 1998.

<http://geosci.uchicago.edu/Faculty/ABBATT/abbatt.html>

<http://rainbow.uchicago.edu/chemistry/fac/butler.html>

b. Preprints

Nickel Deposition on Silicon Surfaces

Proceedings of the Society of Photo-Optical Instrumentation Engineers

Cs. Beleznai, L. Nanai, S. Leppavuori, J. Remes, H. Moilanese and Thomas F. George*

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

Nickel deposition is carried out by scanning an Ar⁺ laser beam on Si surfaces in an atmosphere of Ni(CO)₄, and a theoretical analysis is presented.

Ripple Formation on GaAs Surfaces by Ultrafast (fs) Laser Pulses

Proceedings of the Society of Photo-Optical Instrumentation Engineers

L. Nanai, R. Vajtai, L. Fabian, S. Szatmari, S. Leppavuori and Thomas F. George*

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

Optical and atomic force microscopy studies reveal a double-wavelength character of ripples inside and outside the illuminated areas, and Raman investigations show the existence of zinc-blende to cubic transitions in the crystalline symmetry at the peripheral part of the irradiated area.

Polarization and Dissociation of Excitons in Luminescent Polymers

Synthetic Metals

X. Sun, L. Li, R. L. Fu and Thomas F. George*

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

It is shown that excitons in polymers can possess a very large polarizability, and when the electric field is strong enough, an exciton in luminescent polymers dissociates into a pair of charged polarons.

Second-Sound Attenuation by a Quantized Vortex in a Rectangular Vessel Containing Liquid Helium

Journal of the Korean Physical Society

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

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

Using the linearized equations of superfluid hydrodynamics, the wave equation, dispersion relation and second-sound coefficient are obtained for a rectangular vessel having a quantized vortex.

An analytical potential energy surface of the HCIF (2A_1) system based on ab initio calculations.

Variational transition state theory study of the $H + ClF \rightarrow F + HCl$, $Cl + HF$ and $F + HCl \rightarrow Cl + HF$ reactions and their deuterium isotope variants. Physical Chemistry Chemical Physics (special issue on "Chemical Reaction Theory") submitted.

R. Sayos, J. Hernando, J. Hijazo and Miguel Gonzalez

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

A new analytical PES (2A_1) based on ab initio (PUMP2/6-311G(3d2f,3p2d)) calculations (about 3400 points) is derived for the study of the $H(^2S) + ClF$ (both channels) and the $F(^2P) + HCl$ reactions. Calculated variational transition state theory rate constants with the inclusion of a microcanonical optimized multidimensional tunneling correction are in good accord with experiments at different temperatures, also for the corresponding deuterated reactions

Exact Solution of Two-State Time-Independent Coupled Schroedinger Equations in an Exponential Model

Phys. Rev. A

V. I. Osherov and H. Nakamura*

Department of Theor. Studies, Inst. Molec. Sci., Okazaki 444-8585, Japan

Exact solution for a exponential model in which the exponent of diabatic coupling is one half of that of diabatic potential. A simple and accurate semiclassical formula is found for nonadiabatic transition probability.

Quantum Reaction Dynamics of Asymmetric Exoergic Heavy-Light- Heavy System: $Cl + HBr \rightarrow HCl + Br$

PCCP

G. V. Mil'nikov, O. I. Tolstikhin, K. Nobusada, and H. Nakamura*

Department of Theor. Stud. Inst. Molec. Sci., Okazaki 444-8585, Japan

The concepts of potential ridge and nonadiabatic transitions at avoided crossings introduced previously are confirmed to be useful to clarify the mechanisms of vibrationally nonadiabatic reactions in this exo-(or endo-)ergic system. The role of important avoided crossings which dominate the reaction dynamics is illustrated.

Patterns of Time Propagation on the Grid of Potential Curves

Phys. Rev. A

V. N. Ostrovsky and H. Nakamura*

Department of Theor. Stud. Inst. Molec. Sci., Okazaki 444-8585, Japan

Time-propagation patterns are studied for a network formed by two bands of equidistant rectilinear parallel diabatic potential curves that cross each other. In the case of weak coupling between the bands the propagation proceeds mostly via a diabatic path. In the strong coupling case antidiabatic propagation is revealed.

Multiphoton Excitation

Encyclopedia of computational chemistry(Wiley)

Martin Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

General review

Statistical Adiabatic Channel model

Encyclopedia of Computational Chemistry(Wiley)

Martin Quack and Juergen Troe

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

General review

High resolution cavity ring down absorption spectroscopy of nitrous oxide and chloroform using a near infrared cw diode laser

Chem. Phys. Lett. 1998

Y. He ,M. Hippler ,and M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

MHz instrumental band width achieved using newly developed method

Spectroscopy and Quantum Dynamics of Hydrogen Fluoride Clusters

Advances in Molecular Vibrations(JAI Press 1998) vol 3

Martin Quack and Martin Suhm

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Review of title subject

Ab initio calculations of the structure, kinetics and IR - laser chemical reaction dynamics of fluorooxirane

J. Phys. Chem. (1998)

T.K. Ha, J Pochert, and M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Competitive reaction pathways found by us experimentally are analyzed theoretically

Ab initio calculation of molecular energies including parity violating interactions

J.Chem. Phys(1998)

A. Bakasov, T.K. Ha, M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

A new approach to electroweak quantum chemistry leads to order of magnitude larger values for parity violating potentials in chiral molecules than previously believed.

Inversion Tunneling in aniline from high resolution infrared spectroscopy and quantum theory

Z. Physik. Chem(1998)

B. Fehrensen, D. Luckhaus, M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Mode selective inversion dynamics in aniline

Vibrational Spectroscopy, anharmonic resonances and intramolecular vibrational redistribution in tetrafluoro-iodoethane

Mol. Phys.(1998)

J. Pochert and M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092

Zuerich, Switzerland

Influence of chirality on IVR in the CH infrared chromophore

Global analytical potential hypersurfaces for large amplitude nuclear motion and reaction in methane: I. Formulation of the potentials

J. Chem. Phys 1998

R. Marquardt, M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Formulation and adjustment of a 9 dimensional analytical potential

A new six dimensional analytical potential up to chemically significant energies for the electronic ground state of hydrogen peroxide

J. Chem. Phys.(1998)

B. Kuhn, T.R. Rizzo, D. Luckhaus, M. Quack, and M. Suhm

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Formulation and adjustment of an analytical potential to new ab initio and experimental data

Isotopomer selective overtone spectroscopy by ionization detected IR+UV double resonance of jet cooled aniline

Chem. Phys. Lett.(1998)

B. Fehrensen, M. Hippler, and M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

We have used our new technique of mass and isotope selective infrared spectroscopy to measure quantum stereomutation in chiral aniline -NHD and its inhibition by NH stretching excitation, as well as IVR processes.

Representation of parity violating potentials in molecular main chiral axes

(submitted)

A. Bakasov and M. Quack

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

New concept to study tensor of parity violating energies and comparison of various new techniques for the examples of H_2O_2 and H_2S_2

Ab initio calculation for the anharmonic vibrational resonance dynamics in the overtone spectra of the coupled OH and CH chromophores in CD_2H-OH

(submitted)

M. Quack and M. Willeke

Lab. for Physical Chemistry, ETH Zuerich (Zentrum) CH 8092 Zuerich, Switzerland

Analysis of IVR via direct and indirect pathways

Nuclear spin conversion in CH_3F at elevated temperatures

Phys. Rev. A 57 (1998) 4322-26

B. Nagels, P. Bakker, L.J.F. Hermans and P.L. Chapovsky

Huygens Lab., Leiden University, P.O. Box 9504, 2300RA Leiden, The Netherlands

Spin-conversion measurements on the C-12 and C-13 isotopic species of CH₃F between 300 and 600 K are found to be in agreement with the mixing-of-states model; above 600K an as yet unidentified mechanism seems to be effective.

Direct optical enrichment of nuclear spin conversion of molecules

Chem. Phys. Lett.

L.V. Il'ichov, L.J.F. Hermans, A.M. Shalagin and P.L. Chapovsky

Institute of Automation and Electrometry, Russian Academy of Sciences, 630090 Novosibirsk, Russia

A direct enrichment method for nuclear spin isomers of polyatomic molecules is proposed.

Violation of nuclear-spin symmetry in collisions of symmetric tops

Chem. Phys. Lett. 294 (1998) 387-90

B. Nagels, P. Bakker, L.J.F. Hermans

Huygens Lab, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

In collisions with Oxygen, gaseous CH₃F is found to exhibit direct nuclear spin conversion with an extremely small cross section of $6 \cdot 10^{-26}$ cm², being some 10 orders of magnitude smaller than typical gas-kinetic cross sections.

Nuclear Spin Conversion in Polyatomic Molecules

Annual Rev. Phys. Chemistry

P.L. Chapovsky and L.J.F. Hermans

Huygens Lab., Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

A review is given of recent progress in the field of the separation and the relaxation mechanism of nuclear-spin isomers.

Hyperspherical coordinates for chemical reaction dynamics

Advances in Quantum Chemistry

V. Aquilanti, G. Capecchi and S. Cavalli.

Dipartimento di Chimica, Universita' di Perugia. I-06123 Perugia, Italy.

High Order Harmonic Generation by One and Two Electron Molecular ions in Intense Laser Pulses

Phys. Rev. A

A.D. Bandrauk, H. Yu

Laboratoire de Chimie Theorique, Universite de Sherbrooke, Que, J1K 2R1, Canada

Numerical solutions of the time-dependent Schroedinger equation for the one and two electron ions H₃²⁺, H₃⁺, H₄³⁺, H₄²⁺, H₅⁴⁺, H₅³⁺, have been obtained in short ($t < 50$ fs) intense ($I > 10^{14}$ W/cm²) laser pulses in order to study the role of electron-electron interactions on high order harmonic generation, into the X-Ray region. One electron systems are found to generate harmonics with maximum energy $IP + 6 U_p$ whereas two electron systems give maximum photon energies $IP + 12 U_p$, where IP is the ionization potential and U_p the ponderomotive energy. These high photon energies are produced by electron-electron and nuclear collisions.

Laser-induced Alignment Dynamics of HCN: Permanent Dipole and Polarizability Effects.

Phys. Rev. A

C.M. Dion, A.D. Bandrauk

Labo de Chimie Theorique, Universite de Sherbrooke, Que, J1K2R1, Canada;

A. Keller, O. Atabek, Labo de Photophysique

Moleculaire, Orsay, 91405, France.

The alignment dynamics of HCN in intense ($I=10^{13}$ W/cm²) IR laser pulses are studied numerically by exact solution of the molecular time-dependent Schroedinger equation with ab-initio permanent dipole and polarizability moments. The results are compared to analytic models of a laser driven rigid rotor.

Reactive Scattering of Oxygen and Nitrogen Atoms

Acc. Chem. Res.

P. Casavecchia*, N. Balucani, M. Alagia, L. Cartechini, G.G. Volpi
Dipartimento di Chimica, Università di Perugia, 06123 Perugia, Italy

Natural Alignment and Cooling in Seeded Beams: Experiments and a Quantum Mechanical View

Proceedings of the 21st Rarefied Gas Dynamics.

V. Aquilanti, D. Ascenzi, D. Cappelletti, M. de Castro, F. Pirani
Università di Perugia, Perugia, Italy

Collisional alignment is by itself an important issue of gas dynamics: after providing the proper background by analyzing the relevant experimental information, in this paper we present a discussion of the gas dynamics in terms of extensive quantum mechanical calculations of scattering cross sections and outline recent applications to scattering experiments providing information on intermolecular forces

Quantum Interference Scattering of Aligned Molecules: Bonding in O₄ and role of spin coupling

Phys. Rev. Lett.

Vincenzo Aquilanti, Daniela Ascenzi, Massimiliano Bartolomei, David Cappelletti[†], Simonetta Cavalli, Miguel de Castro Vitores, Fernando Pirani
Università di Perugia, Perugia, Italy

Molecular beam experiments on collisions between oxygen molecules were performed at low energy and high angular resolution, with the control of the relative orientation of the colliding molecules. Dependence on relative orientations for the ground singlet state surface and for the excited triplet and quintet states is obtained. These results indicate that most of the bonding in the dimer comes from electrostatic (van der Waals) forces but chemical (spin-spin) contributions in this open-shell–open-shell system are not negligible.

c. Conferences

1. Winter-School and Workshop on Resonance Phenomena in Chemical Physics

Technion City, Haifa, Israel, February 14 - 19, 1999

Program and Registration form: <http://www.technion.ac.il/technion/chemistry/IASTC/Mo/>

List of invited speakers:

Resonance Definitions and their Fingerprints in Observal Quantities (minicourses): Vitali Averbukh, Erkki Brandas, Eric Heller, Jrgen Korsch, William Miller, Nimrod Moiseyev, Howard Taylor, Ilya Vorobeichik
Different Computational Methods and Algorithms for Calculating Resonances: Claude Leforestier, Vladimir Mandelshtam, Danny Neuhauser, Hans-Dieter Meyer

Theory of Resonance Phenomena in Chemical Physics: Lorenz Cederbaum, Stavros C. Farantos, R. B. Gerber, Peter Hanggi, Georges Jolicard, Pavel Jungwirth, Roland Lefebvre, Claude Leforestier, Evgueni Nikitin, Uri Peskin, Eli Pollak, Moshe Shapiro

Experimental Manifestation of Resonance Phenomena: Eli Kolodney, Ron Naaman, Mark G. Raizen, Hana Reisler, Dan Ritter, Curt Wittig, Daniel Zajfman.

Discussion: Theoretical Interpretation of the Experimental Results: Philip R. Certain

2. WINTER-WORKSHOP "REACTION DYNAMICS"

Mariapfarr, Austria, 16 to 19 February 1999.

The annual Winter-Workshop of the Austrian Chemical Society in Mariapfarr (a resort in the Austrian Alps) will take place from The 1999 workshop is dedicated to "Reaction Dynamics". Lectures will be given by G.G. Balint-Kurti (Bristol), G.D. Billing (Copenhagen), R. Jaquet (Siegen) and U. Manthe (Freiburg). The workshop language is English.

For the full program, for details about the workshop and about Mariapfarr, and for all matters concerning registration, please visit the Mariapfarr-Homepage on http://www.kfunigraz.ac.at/tchwww/sax/mariapfarr/index_eng.html

3. THE 5th GORDON CONFERENCE ON GAS PHASE ION CHEMISTRY

Ventura, California, Feb. 28 - March 5, 1999

The 5th Gordon Conference on Gas Phase Ion Chemistry will be held in Ventura, CA on Feb. 28 - March 5, 1999 The full conference program is now on the web at:

<http://www.unc.edu/depts/chemistry/gordon/index.html>

If this conference is of interest to you, please add this address to your bookmarks.

Tomas Baer, Conference Chair, Kenan Professor of Chemistry, Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290, Baer@unc.edu, <http://net.chem.unc.edu/faculty/tb/cftb01.html>

4. WORKSHOP ON "TIME-DEPENDENT QUANTUM MOLECULAR DYNAMICS"

The Henry Eyring Center for Theoretical Chemistry at the University of Utah and the Quantum Theory Project at the University of Florida wish to announce a workshop on "Time-Dependent Quantum Molecular Dynamics", to be held in beautiful Brian Head, Utah, March 13-17, 1999. At this time, there is space for 20 more attendees, in addition to the invited speakers and their selected graduate students/postdocs. More information on the workshop and a registration form may be found at the web site:

<http://www.hec.utah.edu/brianhead/>.

Please download the registration form and mail it to me at the address below if you are interested in attending.

This workshop should prove to be a very stimulating meeting focused on a topic which has emerged as one of the central themes in theoretical chemistry.

5. American Chemical Society

Anaheim, California, March 21-25, 1999

The following list gives the symposia that are planned for the Anaheim, California meeting of the American Chemical Society (March 21-25, 1999). Abstracts are due November 1, 1998. If you have a contribution that belongs to one of the symposium topics, please send it to one of the organizers of the symposium. Abstracts on other topics should be sent to me. These will be included in a general poster session. Further information concerning this meeting and about other activities of the physical division can be seen at

<http://hackberry.chem.niu.edu/PHYS>

Four copies of 150-word abstract (original on ACS Abstract Form) to symposium organizer by November 1, 1998. Forms are available from <http://www.acs.org>

Linear Polyene Spectroscopy: A Celebration of the Scientific Career of Bryan Earl Kohler, B. S. Hudson, Dept. of Chemistry, Syracuse Univ., Syracuse, NY 13244-4100, (315) 443-5805, fax (315) 443-4070, email: bshudson@syr.edu

Unimolecular Reactions and Intramolecular Dynamics, S. J. Klippenstein, Dept. of Chemistry, Case Western Reserve University, Cleveland, OH 44106; 216-368-6916, fax (216) 368-3006, email: sjk5@po.cwru.edu, David Perry, Department of Chemistry, University of Akron, Akron, OH 44325, (216) 972-6825, fax (216) 972-6990, email: DPerry@uakron.edu

Heavy Element Complexes: The Convergence of Theory and Experiment, (Joint with NUCL), James V. Beitz, Chemistry Division, Argonne National Laboratory, Argonne IL 60439, (630)252-7393 email: beitz@anlchm.chm.anl.gov; David L. Clark, G. T. Seaborg Institute, Mail Stop E500, Los Alamos National Laboratory, Los Alamos, NM 87545, email: dlclark@lanl.gov

Radicals in Condensed Phases, David Bartels, Chemistry Division, Argonne National Laboratory, Argonne IL 60439, (630)252-3485 fax: (630) 252-4993 email: bartels@anlchm.chm.anl.gov; Greg Schenter,

Environmental Molecular Science Lab, MS K1-96, Pacific Northwest National Laboratory, Batelle Blvd, Richland, WA 99352, (509) 375-2945, email: gk_schenter@pnl.gov

Physical Chemistry of Sol-gel Materials, Jeff Zink, Department of Chemistry and Biochemistry, University of California, 405 Hilgard Ave., Los Angeles, CA 90095-1569, 310-825-1001, fax 310-206-9880, zink@chem.ucla.edu; Bruce Dunn, Department of Materials Science and Engineering, UCLA, Los Angeles CA 90095, 310-825-1519, email: dunn@seas.ucla.edu

Dynamics/Structure at Electrochemical Interfaces by New Spectroscopic Probes and Approaches, Andrzej Wieckowski, Chemistry Department, University of Illinois, Urbana, IL 61801, (217)333-7943, fax: (217)333-0711 email: andrzej@aries.scs.uiuc.edu; Joseph T. Hupp, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, (847)491-3504, fax (847)491-7713, email: jthupp@chem.nwu.edu
Liquids and Interfaces (in honor of Doug Henderson), Randall Shirts Department of Chemistry, Brigham Young University, Provo UT 84602-5700, 801-378-4290, fax: 801-378-5474, email: rbshirts@chemdept.byu.edu

Frontiers of Statistical Mechanics (in honor of Ben Widom), A.D.J. Haymet, Department of Chemistry and Institute for Molecular Design, University of Houston, 4800 Calhoun, Houston, TX 77204-5641, 713-743-2781, fax: 713-743-2709 email: haymet@uh.edu

6. Rovibrational Bound States in Polyatomic Molecules

Aberdeen, UK, 11-14 April 1999

This specialist workshop is sponsored by CCP6 (the UK Collaborative Computational Project on Heavy Particle Dynamics). The meeting will focus on the challenging problems associated with wide amplitude rovibrational bound state calculations in tetraatomic molecules and larger. Topics covered will include: coordinate systems; derivation of exact kinetic energy operators; representation of potential energy surfaces; choice of basis functions; strategies such as the discrete variable representation and contraction schemes; large matrix diagonalisation methodologies; and opportunities offered by supercomputer architectures. We intend to limit participation to about 30 keenly interested people, with 12 invited talks. The format will be "Gordon Conference style", with sessions in the morning and evening but afternoons free.

Invited speakers will include:

Zlatko Bacic (USA), Tucker Carrington (Canada), David Clary (UK), Benny Gerber (Israel), Nicholas Handy (UK), Lauri Halonen (Finland), Claude Leforestier (France), Kevin Lehmann (USA), David Nesbitt (USA), Jonathan Tennyson (UK), Ad Van der Avoird (Netherlands)

Organising committee: Mark Law, e-mail: M.M.LAW@ABDN.AC.UK, Jeremy Hutson, Ian Atkinson, For further information please consult the conference Web page
<http://www.abdn.ac.uk/~che194/research/rovib99/>

7. International Symposium on The Treatment of Complex Chemical Systems: New Concepts in Theory and Experiment in honor of Professor Jürgen Brickmann on the occasion of his 60th birthday Department of Chemistry, Darmstadt University of Technology, May 27 - 29, 1999

Scope of the Symposium: Large and complex systems provide some of the most challenging experimental and theoretical problems in modern chemistry. By complex systems, it is meant that the systems as well as the models used should reflect chemical conditions in a realistic way. This requires the proper and simultaneous treatment of different species and phases. The purpose of this symposium is to survey recent research in the development of new model scenarios, new theoretical approaches and simulation techniques of complex systems and processes as well as subtle experimental techniques in order to study these kinds of systems.

It is the aim of this meeting to discuss various ways to overcome the limitations of individual methods by combining different approaches and to demonstrate in this way the power of new concepts and technologies. The invited speakers are selected from a wide variety of fields ranging from philosophy to preparative

chemistry. Therefore, the meeting is expected to be of interest to both experimentalists and theorists from all branches of science, as well as mathematicians and computer scientists.

D. Avnir, Jerusalem (Israel); V. Aquilanti, Perugia (Italy); H. Baumgärtel, Berlin (Germany); R.S. Berry, Chicago (USA); P. Bopp, Bordeaux (France); E. Braendas, Uppsala (Sweden); L. Cederbaum, Heidelberg (Germany); B. Gerber, Jerusalem (Israel); E. Gudowska-Nowak, Krakow (Poland); R. Kniep, Darmstadt (Germany); G. Kothe, Freiburg (Germany); H. Kubinyi, Ludwigshafen (Germany); R. D. Levine, Jerusalem (Israel); H. Limbach, Berlin (Germany); P. Mezey, Saskatchewan (Canada); J. Mittelstrass, Konstanz (Germany); K. Schulten, Urbana-Champaign (USA); A. Sgamellotti, Perugia (Italy); A. Skerra, Darmstadt (Germany); J. Weber, Geneva (Switzerland); E. Yurtsever, Istanbul (Turkey);

Registration fee: none. Hotel rooms can be reserved by contacting the tourcongress bureau Darmstadt, Luisenplatz 5, D-64283 Darmstadt, phone: (+49) 6151-13 20 7, fax: (+49) 6151-13 20 75 Please register on-line at: <http://www.pc.chemie.tu-darmstadt.de/symposium1999/>

Please send correspondence to: Dr. Hans-Jürgen Bär, Institute of Physical Chemistry, Darmstadt University of Technology, Petersenstr. 20, D-64289 Darmstadt, Germany, Fax: (+49) 6151/164298, Email: hjb@pc.chemie.tu-darmstadt.de

8. 18th International Symposium on Molecular Beams 1999

Ameland, The Netherlands, May 30 - June 4, 1999

Chairmen: Steven Stolte (VU Amsterdam) and Gerard Meijer (KU Nijmegen)

A Web-page is being prepared and will be announced in the next issue of MDN and on the department home-page: <http://www-mlf.sci.kun.nl/mlf/>

9. XVI INTERNATIONAL CONFERENCE ON MOLECULAR ENERGY TRANSFER (COMET XVI)

"La Cittadella", Assisi, ITALY, June 20-25, 1999

<http://www.chm.unipg.it/chimgen/mb/cong/comet.html> e-mail: comet@dyn.unipg.it

The XVI International Conference On Molecular Energy Transfer, COMET XVI, will be held at "La Cittadella", a conference facility in Assisi, ITALY, 20-25 June 1999. Assisi is a unique medieval town rich in art masterpieces. It is located in a beautiful landscape, 25 km east of Perugia, the capital of the Umbria region known as the "green heart" of Italy. The COMET is a Gordon type conference held every two years alternating between the USA and Europe.

The purpose of the 1999 conference is to survey recent advances, undertake stimulating discussions, generate new ideas, and map out future directions in the field of molecular energy transfer. The scientific program will concentrate on dynamical aspects of molecular energy transfer. Particular emphasis will be given to

State-to-state dynamics

Inelastic and reactive collisions

Unimolecular reactions

Ion reaction dynamics

State-selected (inter- and intra-molecular) energy transfer

Internal vibrational redistribution

Energy transfer in condensed phase

Clusters and hydrogen bonded systems

Photodissociation

Imaging techniques

Non-adiabatic processes

Open-shell dynamics and spectroscopy

Transition state spectroscopy

Femtosecond dynamics

INVITED SPEAKERS

M.H. Alexander (University of Maryland), M.N.R. Ashfold (University of Bristol), G. Balint-Kurti (University of Bristol), J.M. Bowman (Emory University), D.C. Clary (University College London), F.F. Crim (University of Wisconsin), O. Dutuit (Universit de Paris-Sud, Orsay), G.R. Fleming (University of California, Berkeley), G.W. Flynn (Columbia University), D.R. Herschbach (Harvard University), F. Huisken (Max-Planck-Institut, Goettingen), M.I. Lester (University of Pennsylvania), J.C. Light (University of Chicago), W.C. Lineberger (JILA, University of Colorado), K. Liu (IAMS, Academia Sinica, Taipei), H.H.J. ter Meulen (University of Nijmegen), W.H. Miller (University of California, Berkeley), E. Murad (Air Force Research Lab, Hanscom AFB), R. Naaman (Weizmann Institute, Rehovot), D. Nesbitt (JILA, University of Colorado), D.M. Neumark (University of California, Berkeley), G.A. Parker (University of Oklahoma), H. Reissler (University of Southern California), G. Scoles (Princeton University), J.P. Simons (Oxford University), T. Suzuki (IMS, Okazaki), F. Vecchiocattivi (University of Perugia), R.N. Zare (Stanford University),

Piergiorgio Casavecchia (Co-Chair), Dipartimento di Chimica, Universit di Perugia, 06123 Perugia, Italy, Phone: (+39) (075) 585-5514, Fax: (+39) (075) 585-5606, Email: piero@dyn.unipg.it

Antonio Lagana' (Co-Chair), Dipartimento di Chimica, Universit di Perugia, 06123 Perugia, Italy, Phone: (+39) (075) 585-5515, Fax: (+39) (075) 585-5606, Email: lag@dyn.unipg.it

The local organizing committee includes the members of the Perugia Group: V. Aquilanti, N. Balucani, B. Brunetti, R. Candori, D. Cappelletti, S. Cavalli, S. Crocchianti, S. Falcinelli, G. Grossi, G. Liuti, E. Luzzatti, F. Pirani, F. Vecchiocattivi, G.G. Volpi.

Note that COMET XVI will be followed immediately after by the "Workshop on Quantum Reactive Scattering" (Perugia, Italy, 25-27 June 1999) and by the 1st European Computational Chemistry School on "Molecular and Reaction Dynamics" (Perugia, Italy, June 28-July 4, 1999).

Information will be continuously updated on the Web site. On January 1999 it will be e-mailed to people on the Conference mailing list. To be added to the mailing list, please fill out the form and mail or fax it. You can also pre-register at our Web Site: <http://www.chm.unipg.it/chimgen/mb/cong/comet.html>

The Second Announcement will include more specific details about the call for papers, registration, fees, traveling and housing.

PRE-REGISTRATION FORM

To receive further information, register at our WWW site

<http://www.chm.unipg.it/chimgen/mb/cong/comet.html> or return this slip (e-mail, fax, or regular mail) before January 15, 1999.

Last Name:

First Name:

E-mail:

Phone:

Fax:

Address:

If you are unable to access our WWW site, please check here ____ to receive a hard copy of forthcoming information.

COMET XVI, Prof. P.Casavecchia, Dipartimento di Chimica, Universita' di Perugia, Via Elce di Sotto, 8, 06123 PERUGIA, ITALY

FAX: (39) 075 5855606, e-mail comet@dyn.unipg.it

10. WORKSHOP ON QUANTUM REACTIVE SCATTERING

Perugia, Italy, 25-27 June, 1999

The meeting, which will be sponsored by the D9 COST Action in Chemistry, will hopefully be attended by most of the world experts in the field, and will be run in the same spirit and with the same objectives as the

four previous workshops on reactive scattering (Cambridge UK, 1990, organised by David Clary, Cambridge USA, 1994, organised by Yan Sun and Michael Baer, Nottingham UK, 1995, organised by David Clary and David Manolopoulos, and Telluride, Colorado, 1997, organised by Joel Bowman).

The emphasis of the workshop will be on the latest theoretical developments and the most impressive recent calculations. The most ingenious new approximations in reactive scattering will also be discussed.

Interesting new directions for the application of reactive scattering theories will also be discussed, with special attention towards systems of increasing complexity, according to the aims of the D9 COST Action. For information, contact V. Aquilanti [aquila@dyn.unipg.it] or A. Laganà [lag@dyn.unipg.it]

11. EUROPEAN COMPUTATIONAL CHEMISTRY SCHOOL: MOLECULAR AND REACTION DYNAMICS

Perugia, Italy, June 28 - July 4, 1999

The European Computational Chemistry Groups have started a European School on "Molecular and Reaction Dynamics" to be held in Perugia (Italy) every fourth year starting from its first edition (June 28 - July 4, 1999). The School will be jointly run by the Department of Chemistry and the Computer Center of the University of Perugia.

Morning sessions will be devoted to chemical theory and problems while the afternoon sessions will be devoted to Computer Science advances and Computational Chemistry applications (two plenary lectures dealing with fundamental aspects of reactivity and dynamics calculations of molecular systems during the morning session; one lecture on computing advances and a three hour long tutorial devoted to Molecular and Reaction Dynamics computational applications in the afternoon).

Have already accepted to deliver lectures G.C. Schatz, M. Vanneschi, G.A. Parker, A. Kupperman, G.G. Balint Kurti, J. Zhang, D. Kouri, G.D. Billing, M. Robb, F. Bernardi.

For further information contact Prof. Antonio Lagana'

Dipartimento di Chimica, Università di Perugia, Perugia (Italy),

email lag@unipg.it,

tel. +39.75.5855515, tel. +39.75.5855606.

Information will also appear soon in the web (www.chm.unipg.it/chimgen/mb/theol/gicc.html)

12. THE 1999 AMERICAN CONFERENCE ON THEORETICAL CHEMISTRY (ACTC)

Boulder, June 27-July 2 1999

Information: Prof. Eric Heller

heller@physics.harvard.edu

13. STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS

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

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

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

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

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

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

- * Demonstrations of active or coherent control of chemical processes

At this time we are seeking Titles and Abstracts of about 300 words. The DEADLINE for submission of these proposed contributions is FRIDAY 29 MAY 1998. They should be sent to Dr. BJ Whitaker, School of Chemistry, University of Leeds, LS2 9JT and may be in any form - manuscript, fax, whatever but electronic

attachments will be particularly cherished. Papers should be concerned with new, unpublished work. The full proceedings of the Discussion will be published late in 1999, but papers accepted for discussion will be circulated to all participants before the meeting in July 1999. Those unfamiliar with the unique format of Faraday Discussions can obtain more information from the URL above.

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

14. THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE

Split Rock Resort in Lake Harmony, Pennsylvania, USA, July 18-23, 1999

James J. Valentini, Chair, 1999 Dynamics of Molecular Collisions Conference

15. ICPEAC XXI

July 22 - 27, 1999, Sendai, Japan

The twenty first meeting of the International Conference on the Physics of Electronic and Atomic Collisions will be held July 22 - 27, 1999 (Thursday - Tuesday) in Sendai, Japan. Sendai is the economic and cultural center of the Tohoku (north- eastern) region of Japan. It is located near the ocean 200 miles north of Tokyo. Further information may be obtained from Prof. Michio Matsuzawa, Applied Physics & Chemistry, University of Electro-Communications, Tokyo, 182-8585, Japan. Fax: 81-424-43-5505 e-mail michio@pc.uec.ac.jp Homepage: <http://power1.pc.uec.ac.jp/Sendai>

16. PHOTO-DYNAMICS AND REACTION DYNAMICS OF MOLECULES

Inst. for Molec. Science, Okazaki, Japan, July 31(Sat) - August 2(Mon), 1999.

Organizers: Hiroki Nakamura and Koichiro Mitsuke, Inst. Molec. Sci., Okazaki. e-mails: nakamura@ims.ac.jp, mitsuke@ims.ac.jp, Home page: <http://www.ims.ac.jp/pdrdm/>

Scope of the symposium

This satellite meeting of The XXI ICPEAC in Sendai is primarily intended to exchange scientific information and discussions among scientists who are interested in the studies of dynamics of molecules such as molecular photo-ionization, molecular photo-excitation and dissociation, molecular reaction dynamics, and transition-state spectroscopy. The scientific program will be composed of invited talks, some oral presentations and poster sessions, covering both experimental and theoretical aspects. The invited talks are expected to cover the following broad areas: Inner shell photoionization and subsequent decay dynamics, Multiple ionization and dichroism, Dynamics of superexcited molecules, Excited atom ionization and time-resolved spectroscopy, Photoionization complete experiments, Ionization of oriented molecules, laser investigation of molecular photodissociation, Multiphoton experiments, VUV laser experiments, Reaction dynamics involving excited-state atoms, Dynamical behaviors of molecules in an intense laser field, Reaction of highly-charged ions, Transition-state spectroscopy, Theory of chemical reaction dynamics

17. Gordon Research Conference on: Dynamics at Surfaces

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

Chair: Aart Kleyn FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands Email: KLEYN@AMOLF.NL

Vice-Chair: Bruce Kay Pacific NW Natl Lab, Environm Mol Sci Lab, Richland, WA

The next meeting in this very dynamic series will be held again at Proctor Academy. The meeting will be in the same spirit as the very successful preceding ones, both in the sessions and other entertainment.

Topics of this Gordon Research Conference will include: Adsorption-Desorption, Adsorbate Vibrations, Atmospheric Surface Science, Charge Transfer, Diffusion and Growth, Gas-Surface Scattering, Liquid Surfaces, Nano-Scale Studies and Manipulation, Nano-Tribology, Photo-Dynamics and Chemistry, Surface Reactions and Catalysis, Best Student / Postdoc Poster Talks.

Information concerning the conference can be found at: <http://www.grc.uri.edu/programs/1999/surfaces.htm>

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

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

19. 25th International Symposium on Free Radicals

Flagstaff, Arizona, August 15-20, 1999.

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

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

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

SCIENTIFIC PROGRAM

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

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

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

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

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

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

Oxford, 13 and 14 September 1999

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

Special announcement

SPECIAL MATERIALS

Scientific Opportunities in Chemical Dynamics at the Advanced Light Source.

The Chemical Dynamics Beamline at the Advanced Light Source is a national user facility operated by the Chemical Sciences Division of the US Department of Energy, Office of Basic Energy Sciences. It is available for use by qualified investigators for a broad range of studies including (though by no means limited to) photochemistry, chemical reaction dynamics, and high resolution photoionization and photoelectron spectroscopy and dynamics. The Beamline features the worlds brightest source of continuously tunable VUV light, along with several dedicated molecular beam based endstations, the worlds highest resolution scanning monochromator in the VUV, and a broad range of laser resources. Please examine the beamline web page, <http://www.lbl.gov/chemicaldynamics> for more detailed information on the available resources and gaining access to the facility. Routine experiments, i.e. those requiring little or no modification to the beamline and endstations, may be proposed through 1-2 page white papers. Interested parties should contact Dr. Arthur Suits, agsuits@lbl.gov, for more information.

BOOKS

MOLECULAR COMPLEXES IN EARTH'S, PLANETARY, COMETARY, AND INTERSTELLAR ATMOSPHERES

Edited by: A. A. Viggasin & Z. Slanina

Contents:

Statistical Physics and Thermodynamics of Bimolecular Complexes

Non-rigidity in van der Waals Molecules: Some Case Studies

Dimeric Absorption in the Atmosphere

Dimers in Earth's and Planetary Atmospheres: The $(\text{H}_2\text{O})_2$, $(\text{N}_2)_2$, $\text{N}_2\text{-O}_2$, $(\text{O}_2)_2$, $(\text{O}_3)_2$, $(\text{CO}_2)_2$, $(\text{H}_2)_2$, and Ar- N_2 Cases

Fullerenes and Other Carbon Aggregates, and the Diffuse Interstellar Bands

Planetary Atmospheres: The Role of Collision-induced Absorption

Chemical and Optical Properties of Molecular Complexes Using Matrix Isolation Spectroscopy

Infrared Spectroscopy of Size-selected Free and Adsorbed Water Complexes

Published by: World Scientific, Singapore 1998, ISBN 981-02-3211-X, 288pp.

Booklet available: Molecular Quantum States at Dissociation

We recently organised a CCP6 Workshop on "Molecular Quantum States at Dissociation". CCP6 has now published a booklet containing short reviews by the Workshop participants. Single copies of this are available free of charge (until we run out).

If you would like a copy, please either:

1) Fill in the form on the Web at <http://www.tampa.phys.ucl.ac.uk/mqsd/bookform.html>

2) Send email to ucapcab@ucl.ac.uk including your postal address and a request for the booklet.

An electronic version of the booklet, which is in postscript and therefore rather large (2Mb), is available via <http://www.tampa.phys.ucl.ac.uk/mqsd/booklet.html>

NEW JOURNAL

There is a new, purely electronic journal published by the Royal Society of Chemistry: "PhysChemComm" which offers an exciting new approach to the communication of research in physical chemistry.

The choice of name is motivated by reference to 'Chemical Communications' ('ChemComm') to emphasize its role in providing a high impact, very rapid publication journal, though not necessarily of short communications. It is a broad spectrum journal embracing all areas of Physical Chemistry and the topics which border upon it. Its founding Editors are Paul Madden (Oxford), Paul Alivisatos and Graham Fleming (Berkeley), assisted by Godfrey Beddard (Leeds) and John Simons (Oxford). It is organised through the Royal Society of Chemistry's Editorial Office. Please look at the web site of this new journal: <http://www.rsc.org/physcc>, where real 'example' papers can already be found.

The development of electronic publishing will, over time, change the ways in which we publish and disseminate our work, and the goal of the Royal Society of Chemistry and "PhysChemComm" is to be the leading e-journal in this new area. In our own research groups and at scientific meetings, breakthrough results are now routinely presented in ways that are poorly compatible with conventional publication. Videos of dynamical processes and simulations of chemical transformations are two examples. Color graphs often cost too much to publish in conventional journals, and as a consequence authors settle for black and white, and the publication is diminished in quality. Multidimensional data or surfaces cannot be adequately displayed on paper, but can be rotated or sliced on the computer.

There are many ways available to you to publish results in a conventional format. Here are some of the advantages of "PhysChemComm":

all electronic (from submission to publication) //full backing of the Royal Society of Chemistry for archival maintenance //two referees //rapid publication, typically six weeks from submission //treated by Chemical Abstracts and the ISI (Citation Index) as conventional papers //high quality graphics, including 'movies'; free color publication; multidimensional graphs; inclusion of down-loadable data (e.g. spectra, surfaces); use of links within a paper and to external sites and ultimately, to other publications referenced in the text // straightforward printing using your own net software