

Molecular Dynamics News

numbers 106.107; April, June 2000

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 has been accepted - otherwise state *unpublished*).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 108 to Prof. R. Anderson. (You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU. (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#107). The closing date for issue number 108 is August 1, 2000.

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

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

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

Name: _____

Address: _____

Electronic Mail Address (optional): _____

WWW Address (optional): _____

Fax Number (optional): _____

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

ELECTRONIC DELIVERY OF MDN

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

1. Electronic mail to subscribers

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

2. World Wide Web

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

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

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

All members of the chemical physics community are invited to join the (free) "molecular-dynamics-news" email list. The "molecular dynamics" in the title is to be interpreted as meaning "dynamical processes in molecules" rather than "classical simulations of molecular motion". The list can be used to distribute details of conferences, vacant academic and postdoctoral positions, changes of address and other news in the Molecular Dynamics field. It also serves as an archive of up-to-date email addresses for people in the field. The list was created by Jeremy Hutson in June 1993 and has now more than 1600 members.

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

```
join molecular-dynamics-news John F Kennedy
```

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

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

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

```
review molecular-dynamics-news
```

to the address mailbase@mailbase.ac.uk

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

a. Open Positions

FACULTY

Research Professorship Position

Three Research Professorship Position Available at the State Key Laboratory of Molecular Reaction Dynamics, Institute of Chemistry, Chinese Academy of Sciences at Beijing

Three full research professor positions are available and need to be filled from Jan. 2000 to Dec. 2001, at the State Key Laboratory of Molecular Reaction Dynamics (MRDLAB), Institute of Chemistry, Chinese Academy of Sciences (CAS) at Beijing.

Position title: Full research professor

Starting fund: 2M. RMB/3 years and supporting facilities

Base salary: 4000 RMB/month + fringe benefit

Housing: 3 bedroom apartment

Candidates are expected to have more than two years of research experiences after obtaining Ph.D. degree in Physical Chemistry or (Chemical) Physics. Each of the candidates is expected to be leader of an independent research group in the following three areas:

Femtosecond Laser Chemistry in the following research directions: Ultrafast spectroscopy, Reaction dynamics and mechanism, Electron and proton transfer processes, Energy transfer, internal conversion and solvation processes, etc

Photochemical Dynamics in Condensed & Gas Phase in the following research directions: Reaction dynamics in the liquid phase and gas phase, Isomerization dynamics, Electron transfer in polymer, semiconductor, and biological systems, Other dynamic processes in the condensed phase, etc.

Atomic Clusters and Gaseous Molecules in the following directions: Photoelectron spectroscopy of clusters, ZEKE spectroscopy, Reactivity of atomic clusters and gaseous molecules, Transition state Spectroscopy, Caging effects in clusters, etc.

MRDLAB is one of the few laboratories in China focusing on researches in various areas of modern physical chemistry. It was founded in 1986, with the auspice of Nobel laureate Professor Yuan T. Lee as its honorary director, and with the annual funding support from the State Planning Committee. The MRDLAB is also supported by the Innovation Project of CAS through the newly established Center of Molecular Sciences (CMS) of CAS. Major fundings are also from the State Department of Sciences & Technology and Chinese National Science Foundation. Successful candidates are also going to be supported by the Hundred Person Project of CAS.

The advantages to work at MRDLAB are: Leading research laboratory in China, Well-equipped and with good research support, Close contact with major funding agencies, Close contact with Peking & Tsinghua Universities (walking distance), Good academic research atmosphere, In expanding phase in next few years
For more information please visit MRDLAB homepage at:

<http://159.226.64.133/>

Contact Information:

Please email your CV to:

Professor and Vice Director Gao, Zhen at gaoz@mrdlab.icas.ac.cn (FAX): 86-010-62563167

Or please mail to: Professor & Director Zhen Gao, Molecular Reaction Dynamics Laboratory, Institute of Chemistry, CAS, 1st North St., ZhongGuanCun

HaiDian District, Beijing, People's Republic of China 100080

*Note: The update version of this announcement could be obtained at the Job Announcement section of our homepage at: <http://159.226.64.133/>

Senior Lecturer/Lecturer in Physical Chemistry and Lecturer (Fixed Term) in Physical Chemistry

University of Durham (UK), Department of Chemistry

Senior Lecturer/Lecturer in Physical Chemistry - Salary 17,238 - 35,670

Lecturer (Fixed Term) in Physical Chemistry - Salary 17,238 - 30,065

Two lectureships are available commencing 1 September 2000 or as soon as possible thereafter. Applicants should have a Ph.D. in chemistry or physics and an excellent track record in research in some area of experimental physical chemistry or chemical physics. A strong interest in teaching at undergraduate and graduate level is also required. The successful candidates will be expected to establish an independent research profile at Durham.

[in the UK system, lectureships and senior lectureships roughly correspond to assistant and associate professorships in the US]

The Chemistry Department at Durham has been rated Grade 5 in each of the last two Research Assessment exercises (in 1992 and 1996). Further information on the Department is available at

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

Informal enquiries about the posts (academic only) may be made by email to the Head of Department, Professor J M Hutson (j.m.hutson@durham.ac.uk) or the head of the Physical Chemistry Section, Professor R K Harris (r.k.harris@durham.ac.uk). Further details and an application form may be obtained from the Director of Personnel, University of Durham, Old Shire Hall, Durham, DH1 3HP (answerphone 0191 374 7258, fax 0191 374 7253 or by email from Acad.Recruit@durham.ac.uk).

Closing date 2 May 2000. Reference Number A136C

Temple University, Faculty Positions in Physics

The College of Science and Technology at Temple University is in the process of a major recruitment effort and is filling 34 faculty positions as part of a major expansion. The College invites applications for positions at the level of Full, Associate and Assistant Professor. Newly hired faculty will be given tenure track positions within the Department of Physics. Successful candidates are expected to have, or be able to develop, a significant research program supported by external funding and to have a strong commitment to teaching at both the undergraduate and graduate level. Candidates should also have a strong interest in interdisciplinary collaboration with the other Departments of the College as well as with Research Centers in the College, examples of which include the Center for Biotechnology, Center for Computer Science and Applied Mathematics, Center for Environmental Science and Technology, and the Center for Bioengineering and Biomaterials. In addition to these, new centers are being formed, including a center for advanced research in Physics to promote interdisciplinary collaboration.

Areas of particular interest include but are not limited to

1. high energy nuclear and particle physics,
2. soft condensed matter physics,
3. molecular physics.

Both experimentalists and theoreticians will be considered. Salary will be competitive and commensurate with qualifications and level of appointment.

Candidates should submit a letter of application, curriculum vitae, and a publication list, as well as evidence of teaching skills and a funded research program. They should also arrange to have three letters of reference sent to: Chair, Physics Faculty Search Committee, Office of the Dean, College of Science and Technology, 409 Barton Hall A, Temple University, Philadelphia, PA 19122. Additional information may be obtained at www.temple.edu/physics or by e-mailing meziani@vm.temple.edu. Temple University is an Equal

Opportunity/ Affirmative Action Employer.

Original announcement is available at:

http://www.temple.edu/CST/jobs/Physics_ad_1999-2000.htm

POST DOCTORAL AND VISITING

Postdoctoral Position in Molecular Dications at University College London.

A postdoctoral position is available in the Chemistry Department at UCL to study the formation, reactivity and decay of molecular dications using both experimental and theoretical techniques. The position is available from March 1st 2000 for one year in the first instance with the possibility of renewal for a further 18 months. The position is part of a European Network in Multiply Charged Ions, which is funded by the European Commission as part of the Framework 5 programme. Eligibility is therefore restricted to European nationals who are not UK citizens. The project will be supervised by Dr Stephen D. Price and Dr Nikolas Kaltsoyannis. Further information can be obtained from either Dr Price or Dr Kaltsoyannis at the address given below, or by email to either s.d.price@ucl.ac.uk or n.kaltsoyannis@ucl.ac.uk.

Selected Publications:

- 1 S.D. Price, J. Chem. Soc., Faraday Trans. 93, 2451 (1997).
- 2 Y.Y. Lee, S.R. Leone, P.H. Champkin, N. Kaltsoyannis and S.D. Price, J. Chem. Phys. 106, 7981 (1997).
- 3 P.H. Champkin, N. Kaltsoyannis and S.D. Price, Int. J. Mass Spectr. Ion Proc. 172, 57 (1998).
- 4 P.H. Champkin, N. Kaltsoyannis and S.D. Price, J. Elec. Spectr. Relat. Phenom. 105, 21 (1999).
- 5 N. Tafadar, N. Kaltsoyannis and S.D. Price, Int. J. Mass Spectr. Ion Proc. 192, 205 (1999).
- 6 N. Kaltsoyannis and S.D. Price, Chem. Phys. Lett. 313, 679 (1999).

To apply, please send a copy of your curriculum vitae and two supporting references to either Dr Stephen D. Price or Dr Nikolas Kaltsoyannis at

Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ., UK

Tel 020 7679 4670, International +44 20 7679 4670

Fax 020 7679 7463, International +44 20 7679 7463

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

POSTDOC position, Munich

THEORETICAL REACTION DYNAMICS in the group of Dr. Uwe Manthe Theoretical Chemistry, TU Munich, Germany

A postdoc position is vacant in the group of Dr. Uwe Manthe in Munich. The research of the group focuses on the theoretical reaction dynamics and the development of molecular quantum dynamical methods.

Representative publications are:

F. Matzkies and U. Manthe, "Combined iterative diagonalisation and statistical sampling in accurate reaction rate calculations: rotational effects in $O+HCl \rightarrow OH+Cl$ ", J. Chem. Phys. 112, 130 (2000);

F. Matzkies und U. Manthe, "Accurate quantum calculations of thermal rate constants employing MCTDH: $H_2+OH \rightarrow H+H_2O$ and $D_2+OH \rightarrow D+DOH$ ", J. Chem. Phys. 108, 4828 (1998);

T. Gerdts und U. Manthe, "A microscopic description of dissipation in systems with strong vibronic coupling: the S_1 and S_2 absorption spectra of pyrazine", Chem. Phys. Lett. 295, 167 (1998);

Funding is provided by the EU within the research training network "Reaction Dynamics: Experimental studies on the Dynamics of Reactions of Atoms and Radicals of Fundamental and Practical Importance".

The project includes reaction rate calculations for $OH+HCl$, $OH+H_2$, and H_2+Cl . In addition, the investigations might be extended to larger gas phase systems ($Cl+CH_4$ or Walden inversion reactions as $Br^-+CH_3Cl \rightarrow CH_3Br+Cl^-$), molecule surface reactions, or address to problem of potential energy surface construction.

The applicant should have experience in quantum molecular dynamics or theoretical reaction dynamics.

For more information contact us (preferentially by E-mail) at the address given below.

E-mail: manthe@ch.tum.de

POSTDOCTORAL FELLOWSHIP- Università di Perugia

Applications are invited for a postdoctoral fellowship in Reaction Dynamics/Astrophysical Chemistry under the supervision of Professor Piergiorgio Casavecchia, and funded by the European Union's TMR (Training and Mobility of Researchers) Programme, as part of the TMR Network on "Astrophysical Chemistry: Experiments, Calculations, and Astrophysical Consequences of Reactions at Low Temperatures". This programme involves eight laboratories: University of Birmingham (UK), University College London (UK), University of Goettingen (Germany), Technische Universitat Chemnitz (Germany), University of Rennes (France), Observatoire de Paris, Meudon (France), University of Bordeaux (France), and the University of Perugia (Italy).

The focus in our laboratory is on studies of chemical reaction dynamics using the Crossed Molecular Beams scattering technique with universal mass-spectrometric detection. Investigation of elementary atom(radical)-molecule and atom-radical reactions of relevance to Astrochemistry are being pursued. We exploit the novel capability of generating intense and continuous supersonic beams of important species such as CARBON and NITROGEN atoms, and HYDROXYL (OH) and CYANO (CN) radicals. All these beams have already been successfully tested and employed in crossed beam studies. Experiments are planned on N, C, and CN reactions, as well as on atom-radical reactions as N+OH. More details of the research field, the technique used, and publications may be found at the following site:

<http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html> and details of the Astrophysical Chemistry TMR Network should also be consulted:

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

The position is available immediately for one year (actually 13 months). Salary is about 3000 EURO/month. The exact commencement date is negotiable. The post-doc is expected to spend up to one month each year in another laboratory of the TMR network. Under the terms of the TMR Programme, applicants must be nationals of a Community Member State or a State associated with the TMR Programme (Iceland, Israel, Liechtenstein, Norway). The young researchers must not be nationals of the state in which the participant appointing them is established (i.e., Italy) and must not have carried out their normal activities in that state for more than 18 of the 24 months prior to their appointment.

Experience in reaction dynamics and molecular beams is desirable. Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcomed. Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

<http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html>

POSTDOCTORAL POSITION, UNIVERSITY OF PERUGIA

Applications are invited for a postdoctoral fellowship in REACTION DYNAMICS under the supervision of Professor Piergiorgio Casavecchia, and funded by the European Union's RTN (Research and Training Network) Programme, as part of the Network on "REACTION DYNAMICS: Experimental and Theoretical Studies on the Dynamics of Reactions of Atoms and Radicals of Fundamental and Practical Importance".

This programme involves eight laboratories: University of Perugia (Italy), University of Oxford (Expt) (UK), University of Nijmegen (Netherlands), University of Bielefeld (Germany), University Complutense Madrid (Spain), University of Oxford (Theory) (UK), University of Stuttgart (Germany), Technical University of Muenchen (Germany). The aim of this Network is to improve substantially our knowledge of the dynamics of elementary chemical reactions by combining, in a synergistic effort, state-of-the-art experimental techniques, based on molecular beam and laser spectroscopic methods, with state-of-the-art quantum chemical methods for calculating the potential energy surfaces that describe the reaction studied experimentally, and state-of-the-art quantum and quasiclassical methods for performing computations of scattering properties and thermal rate constants on these surfaces.

The focus in our laboratory is on experimental studies of chemical reaction dynamics using the Crossed Molecular Beams scattering technique with universal mass-spectrometric detection. Investigation of prototype, elementary atom-molecule and radical-molecule reactions will be pursued, for which dynamical

calculations by quasiclassical and/or quantum methods will be carried out by theoretical teams located in other laboratories participating in this Network. We will exploit the capability of generating intense and continuous supersonic beams of chlorine, oxygen, nitrogen, and carbon atoms and of hydroxyl radicals. More details of the research field, the technique used, and publications may be found at the following site: <http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html>

The position (for up to 3 years duration) for young post-doctoral researchers is available from the Fall 2000 although the exact commencement date is negotiable. Experience in reaction dynamics and molecular beams is desirable. Given the strong links between the different groups in the RTN and in the very spirit of the RTN programme, the post-doc is expected to spend at least one month each year in the laboratory of another Network member.

Salary is about 3000 euro/month (before taxes). Under the terms of the RTN Programme, the young researcher applicant (aged 35 years or less) must be a national of a Community Member State or a State associated with the RTN Programme (Bulgaria, the Czech Republic, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). Subject to its final conclusion, the Association Agreement signed with the Swiss Confederation is expected to enter into force on the 01.01.2001). The young researchers must not be nationals of the state in which the participant appointing them is established and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcome.

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universit di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

REACTION DYNAMICS Network - Postdoctoral opportunities

A 4-year "research training network" (RTN) entitled: "REACTION DYNAMICS: EXPERIMENTAL AND THEORETICAL STUDIES ON THE DYNAMICS OF REACTIONS OF ATOMS AND RADICALS OF FUNDAMENTAL AND PRACTICAL IMPORTANCE" has recently been funded by the European Commission in the framework of the specific research and technological development programme "Improving the Human Research Potential and the Socio-economic Knowledge Base" (Fifth Framework Programme of the European Community). The network involves eight laboratories: Universit di Perugia (Italy) - group leader: Piergiorgio Casavecchia (Network Coordinator);

University of Oxford (UK) - group leader: Mark Brouard;

University of Nijmegen (The Netherlands) - group leader: J. J. Ter Meulen;

University of Bielefeld (Germany) - group leader: Peter Andresen;

Universidad Complutense de Madrid (Spain) - group leader: F. J. Aoiz;

University of Oxford (UK) - group leader: David Manolopoulos;

University of Stuttgart (Germany) - group leader: H.-J. Werner;

Technical University of Muenchen (Germany) - group leader: Uwe Manthe.

The aim is to improve substantially our knowledge of the dynamics of elementary chemical reactions by combining, in a synergistic effort, state-of-the-art experimental techniques, based on molecular beam and laser spectroscopic methods, with state-of-the-art quantum chemical methods for calculating the potential energy surfaces that describe the reaction studied experimentally, and state-of-the-art quantum and quasiclassical methods for performing computations of scattering properties and thermal rate constants on these surfaces.

Eight post-doctoral positions (for up to 3 years duration each) for young researchers with theoretical and/or experimental skills in the field of REACTION DYNAMICS will become available after March 1, 2000. Each group participating in the Network will soon advertise his own post-doc position. Informal inquiries are already welcomed at the addresses below.

Under the terms of the RTN programme, the young researcher applicants (aged 35 years or less) must be nationals of a Community Member State or a State associated with the RTN programme (Bulgaria, the

Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia. Subject to its final conclusion, the Association Agreement signed with the Swiss Confederation is expected to enter into force on the 01.01.2001). The young researchers must not be nationals of the state in which the participant appointing them is established and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

Addresses of team leaders participating in the Network:

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universit di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

Dr. Mark Brouard, Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1 3QZ, UK, E-mail: mark.brouard@chemistry.ox.ac.uk (Phone: (+44) 1865-275457; FAX: (+44) 1865 275410).

Prof. J. J. Ter Meulen, Department of Applied Physics, University of Nijmegen, Toernooiveld 1, 6500 GL Nijmegen, The Netherlands, E-mail: htmeulen@sci.kun.nl (Phone: (+31) 24 365 3022; FAX: (+31) 24 365 3311).

Prof. P. Andresen, Fakultat fuer Physik, University of Bielefeld, Universitatstrasse 25, D-33501 Bielefeld, Germany, E-mail: andresen@physik.uni-bielefeld.de (Phone: (+49) 521 106 5450; FAX: (+49) 521 106 2958).

Prof. F. J. Aoiz, Departamento de Quimica Fisica I, Facultad de Ciencias Quimicas, Universidad Complutense de Madrid, Avenida Complutense s/n, 28040 Madrid, Spain, E-mail: aoiz@legendre.quim.ucm.es (Phone: (+34) 91 394 4126; FAX: (+34) 91 394 4135).

Dr. D. Manolopoulos, Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1, 3QZ, UK, E-mail: mano@physchem.ox.ac.uk (Phone: (+44) 1865-275164; FAX: (+44) 1865 275410).

Prof. H.-J. Werner, Institut for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany, E-mail: werner@theochem.uni-stuttgart.de (Phone: (+49) 711 685 4400; FAX: (+49) 711 685 4442).

Dr. U. Manthe, Institut of Theoretical Chemistry, Technische Universitatet Muenchen, Lichtenbergstrasse 4, 85747 Garching, Germany, E-mail: manthe@ch.tum.de (Phone: (+49) 89 289 13610; FAX: (+49) 89 289 28268).

Postdoctoral position, College of William and Mary

I expect to have a postdoctoral position open beginning late summer or early fall. Our research involves theoretical studies in nonlinear dynamics, order and chaos, high-Rydberg states of atoms, and transport properties of nanojunctions. Send applications and letters of recommendation to J. B. Delos, Physics Department, the College of William and Mary, Williamsburg, VA 23187-8795 (e-mail address delos@atoms.physics.wm.edu). William and Mary is an Equal Opportunity/Affirmative Action University.

Theoretical Postdoctoral Appointment, University of Georgia

Theoretical Postdoctoral Appointment in Atomic and Molecular Collisions at the University of Georgia Applications are invited for a postdoctoral position to conduct theoretical research in low-energy ion-atom/molecule collisions. The position is available immediately and the initial appointment is for one year, possibly renewable for a second or more years depending on available funding and progress. Candidates should have a recent Ph.D. in physics, chemistry, or related field. An interest or expertise in low-to intermediate-energy ion-atom/molecule collisions with one or more theoretical methods including quantal or semiclassical MOCC or AOCC is also desirable. The successful applicant will be part of a program to provide accurate atomic data relevant to astrophysics in the form of a database on the WWW in collaboration with the Controlled Fusion Atomic Data Center at Oak Ridge National Laboratory. Inquiries and applications, including a CV, statement of research interests, and the names and addresses of three references, should be addressed (electronically if possible) to:

Prof. Phillip C. Stancil, Department of Physics and Astronomy, The University of Georgia, Athens, GA

30602-2451

E-MAIL: stancil@hal.physast.uga.edu PHONE: (706) 542-2885, FAX: (706) 542-2492

The application deadline is March 31, 2000, but the search will continue until a suitable candidate is identified. The University of Georgia is Equal Opportunity Employer. For additional information see <http://www.physast.uga.edu/~stancil/postdoc.html>

Postdoctoral Research Associate Position, UNIVERSITY OF NEW MEXICO

A postdoctoral position is available in the group of Prof. H. Guo at the Department of Chemistry, University of New Mexico. The research interests of our group include recursive (Chebyshev, Lanczos) methods for solving bound state and dynamical problems in the gas phase, and photo-induced dynamical processes on solid surfaces. The details of our research can be found in our web page (<http://www.unm.edu/~hguo>). The initial appointment is for one year and renewable for the second year, upon mutual agreement. The salary ranges from \$24,000 to \$30,000, depending on experience. Interested applicants should send CV and three letters of recommendation to: Prof. H. Guo, Department of Chemistry, University of New Mexico, Albuquerque, NM 87131. Email: hguo@unm.edu. Phone: 505 277 1716. Fax: 505 277 2609.

Postdoctoral positions, Newly created International Astrophysics Network

We would like to introduce the newly created International Astrophysics Network.

The prime directives of this network are:

- a. to combine the scientific potentials of highly motivated, flexible, and open minded research groups,
- b. to establish goals/research lines investigating and unraveling the role of neutral - neutral reactions in the gas phase of the interstellar medium/planetary atmospheres and extraterrestrial ices,
- c. exchange ideas what experiments/calculations are necessary and of paramount importance to the chemical processing of the ISM and planetary atmospheres,
- d. perform experiments combined with theoretical treatment of these processes in extraterrestrial environments to setup a systematic database on reaction products and involved intermediates,
- e. implement these data into chemical models of various interstellar environments and planetary atmospheres,
- f. guide the search of hitherto unobserved molecules in the ISM and our solar system.
- g. set up a data base to guide future space missions such as cometary matter return probes, Pluto express, Cassini/Huygens in an identification of hitherto unobserved molecules,
- h. categorize hitherto observed interstellar/cometary molecules according to their formation route (solid state versus gas phase; ion-molecule reactions versus neutral - neutral reactions; distinct classes of neutral neutral reactions involving atoms, clusters, radicals),
- i. encourage exchange of scientists between involved groups,
- j. hold periodically informal workshops to advance the science/strategies in this field,
- k. bring this research field into popular science and educational programs of schools.

The network consists of 6 sections:

Section 1 (laboratory experiments): Our group (group 1) performs neutral - neutral reactions relevant to the chemical processing of the interstellar medium and planetary atmospheres. These experiments provide data on the chemical reaction dynamics, energy dependent triply differential cross sections, involved intermediates, and reaction products.

In addition, our solid state machine is involved in neutral atom and low energy (≤ 5 keV) ion bombardments of extraterrestrial ice analogues to investigate the formation of molecules in extraterrestrial ices and on icy surfaces on interstellar grains. C.S. Lee's group at National Central University, Taiwan (group 2) performs ion bombardments of icy systems at higher energies between 5 and 20 keV. The third group (L. d'Hendecourt et al.) is involved in ultraviolet photon irradiation of extraterrestrial ice analogues. These three groups will setup a systematic data base on the reaction products and involved intermediates and thus provide all the experimental data. Section 2 (electronic structure calculations): Electronic structure calculations investigate theoretically gas phase and solid state neutral - neutral reactions. These calculations will give information on the involved potential energy surfaces, reaction products, involved intermediates,

and rotational constants together with vibrational frequencies of reaction products. These calculations are of fundamental importance in multi-atom systems as studies in groups 1 - 3 . Currently, the following groups are involved in this section: Y. Osamura (reactions of CN radicals with unsaturated hydrocarbons); M. Head-Gordon et al. (reactions of C atoms with small molecules of 4 atoms), A. Mebel et al. (reactions of C atoms with intermediate sized molecules of 5 - 10 atoms), H.F. Schaefer/ P.v.R. Schleyer et al. (reactions of C atoms with large molecules >10 atoms; reactions of C₂D/C₂H radicals; reactions of C₂/C₃ clusters with small molecules <4 atoms; reactions of C₆H₅ radicals with unsaturated hydrocarbons).

Section 3 (RRKM studies): The results of sections 1 and 2 will be complemented and extended by (variational) RRKM calculations. This approach will give unprecedented information on absolute rate constants, theoretical reaction products and branching ratios if more than one product is formed. These investigations are performed by J. Peeters et al (Leuven, Belgium) et al (C/C₆H₆ system, CN/C₂D reactions with unsaturated hydrocarbons, C₆H₅ reactions, B reactions).

Section 4 (modeling): Results of sections 1 - 3 (absolute rate constants, reaction products, branching ratios) will be implemented by T. Millar (UMIST, UK) into models of molecular clouds, hot cores, and outflows of AGB stars. These models can predict the formation and abundance of observed/hitherto unobserved molecules in these environments.

Section 5 (observation): Based on sections 1-4, astronomers will search for hitherto unobserved, but postulated reaction products of neutral - neutral reactions in extraterrestrial environments. The key players in these observations are B. Turner (NRAO, USA), Dr. Y.N. Chih (IAA, Taiwan), T. Lee (IAA, Taiwan), C. Lemme (NCU, Taiwan), Y.J. Kuan (NCNU, Taiwan), and Y. Yung (Caltech, USA).

Section 6 (laboratory microwave spectra): Based on sections 1-3, McCarthy et al will record microwave spectra of hitherto unobserved astronomical molecules in the laboratory. These data will provide the rest frequencies necessary for the astronomical search.

<http://po.iams.sinica.edu.tw/~kaiser/network.htm>

Postdoctoral position, Berlin

Within a cooperation between the Humboldt-Universitaet Berlin (AG Prof. W. Rettig) and the Technische Universitaet Berlin (AG Prof. P. Zimmermann) supported by the Volkswagen Stiftung a postdoctoral position is available (Verg. BAT IIa, duration 14 month with possibility of extension). The aim of the project is the detection of electron transfer states of jet cooled molecules and molecule/solvent cluster by means of optical double resonance techniques in the near UV in electric fields. A suitable apparatus at the TU Berlin is ready to for use. Thechnical support is guaranteed. We offer you exciting high end research in a hot spot' of science. Therefore, we look for a dedicated scientist with experimental skills to carry out these sophisticated experiments and to initiate further developments. Experience with narrow-band tunable ring dye lasers and cw-SHG will be helpful. Experience in sub-doppler laser spectroscopy possibly on supersonic molecular beams and good knowledge in the theory of molecular spectra are desired. Further information is available at Dr.E. Heinecke (elke@kalium.physik.tu-berlin.de) or Dr. Ch. Monte (chmo0435@rz.hu-berlin.de). Applications containing the usual documents should be sent until March 15th, 2000 to: Prof. Dr. Wolfgang Rettig, Walther-Nernst-Institut fr physikalische und theoretische Chemie, Humboldt-Universität zu Berlin, Bunsenstr. 1, 10117 Berlin.

Postdoctoral position, Wayne State University

Post-doctoral position is available in the area of molecular dynamics simulations of adhesion, friction, and lubrication. The position involves both the development of methods/algorithms for the simulations and applications to problems of technological importance. Issues to be addressed include: potential energy functions for surfaces and interfaces, relaxation and energy transfer dyanmcis at interfaces, and wear (i.e. chemical reactions) of sliding surfaces. An important component of the research is direct QM/MM dynamics of sliding surfaces. Please contact William L. Hase, Department of Chemistry, Wayne State University, Detroit, MI 48202, USA; email, wlh@traj.chem.wayne.edu. Wayne State University is an equal opportunity employer.

Postdoctoral position, South Korea

Postdoctoral positions are available in the area of experimental surface reaction dynamics:

- (1) ion-surface reactive scattering,
- (2) development of the related instrumentation.

The positions are affiliated with the Center for Ion-surface Reactive Scattering at Pohang University of Science and Technology (POSTECH), South Korea. Qualified candidates should have a Ph.D. degree in Chemistry, Physics, or a closely related field. Experience in surface science or reactive scattering studies is desirable. Interested candidates should send a resume and letters of recommendation to the following address: Professor Heon Kang Department of Chemistry and Center for Ion-surface Reactive Scattering Pohang University of Science and Technology, Pohang, Gyeong-buk, 790-784, South Korea
E-mail: surfion@postech.ac.kr, http://chem.postech.ac.kr/people/faculty/Hkang_2.htm
<http://chem.postech.ac.kr/~surfion/cisr/cisr.htm>

Postdoctoral Teaching/Research Position, Marquette University

A postdoctoral-level teaching/research position is available in the Marquette University Department of Chemistry for 2000-2001. This temporary, 12-month position carries the university rank of instructor and requires a Ph.D. in Physical Chemistry or Chemical Physics. Salary will be commensurate with the position. Expected teaching duties will be the undergraduate physical chemistry lecture course (fall and spring semesters). Participation in research with the Hossenlopp group is also expected with choice of project based on background and interests of the successful candidate. Examples of potential research projects include fundamental studies of photodissociation dynamics of moderate to large size organic carbonyl compounds [J. Am. Chem. Soc. 118, 4181-7 (1996), J. Am. Chem. Soc. 118, 4188-9 (1996), Chem. Phys. Lett. 110, 229-34 (1997)] and laser-assisted chemical vapor deposition of tin oxide thin films for gas-sensor applications [Appl. Organomet. Chem. 11, 147-51 (1997), Appl. Organomet. Chem. 12, 147-54 (1998)]. For further information on this position, please contact me via email (Jeanne.Hossenlopp@Marquette.edu) or phone (414) 288-3537.

Candidates should send a CV, cover letter, and arrange to have two letters of recommendation sent to:
Prof. Jeanne M. Hossenlopp, Marquette University, Department of Chemistry
P.O. Box 1881, Milwaukee, WI 53201-1881

The announcement for this position is posted at: <http://www.marquette.edu/hr/wfmfac.html>

Two post-doctoral positions, University of California, Santa Barbara

Two post-doctoral positions are available immediately in the laboratory of Professor Alec Wodtke at the University of California Santa Barbara. Chemical Interactions of vibrationally excited molecules with metal surfaces.

We are using stimulated emission pumping and overtone pumping to prepare single quantum states of highly vibrationally excited molecules. The excited molecules are carried in a molecular beam through a UHV chamber to a well-characterized surface and we observe scattering and surface sticking. So far, we have concentrated on interactions with clean metal surfaces. In these studies we have found strong evidence for vibration induced electron transfer and we intend to pursue this interesting result further. The project has already resulted in two papers in Science with another in the pipeline. One example of future work is to investigate the vibrational energy transfer to Shottky barrier diodes. Such experiments could directly reveal direct evidence of the electron transfer reaction, taking place at the surface and potentially lead to new laser-based molecular sensors. Another example of future work is the study of state-specific vibration induced surface reactions.

The project is an ongoing collaboration between Alec Wodtke and Daniel Auerbach. It is very well funded with an excellent array of equipment dedicated to the project: presently, three injection seeded Yag-pumped dye laser systems with non-linear optics and a molecular beam surface scattering apparatus. The experiment is quite demanding technically. We seek a person who likes high-tech experimental physical chemistry, has experience with laser spectroscopy and high vacuum equipment. The successful candidate must be independent and self-motivated. We believe this is an excellent opportunity for an ambitious individual to advance his or her career in basic research.

Interested individuals should send an electronic resume including at least two references to: Alec M. Wodtke, Wodtke@chem.ucsb.edu AND Daniel J. Auerbach, Dja@almaden.ibm.com.

Rapid Evaporative Cooling Mass Spectrometry of DNA We are finishing the construction of a custom time-of-flight mass spectrometer as part of an NIH funded study to develop new methods of high-speed gene sequencing. The approach exploits recent observations that molecules ionized from within van der Waals clusters can release large amounts of excess energy by rapid evaporation of weakly bound atoms and molecules. This is found to suppress fragmentation rates in the substrate by more than four orders of magnitude. Successful demonstration of suppressed fragmentation in mass spectrometry of DNA has many important implications. High-speed gene sequencing is one of them. The project is a collaboration between Alec M. Wodtke (physical chemistry and instrumentation) and Norbert O. Reich (an expert on DNA enzymology). It is still at an early stage and thus represents a great opportunity for someone to get in on the ground floor. Experience with any or all of the following: high vacuum methods, instrument design, mass spectrometry, laser desorption, photoionization and electron capture would all be seen favorably; however, we seek an individual who is interested in learning new methods. He or she should have a strong background in experimental physical chemistry but be intellectually flexible enough to learn and carry out experiments in biochemistry and even molecular biology, e.g. polymerase chain reaction, recombinant DNA methods. The successful candidate must be independent and self-motivated.

We believe that this position is an excellent opportunity for someone presently working in an area of experimental physical chemistry to branch out into modern biotechnology.

Interested individuals should send an electronic resume including at least two references to: Alec M. Wodtke, Wodtke@chem.ucsb.edu AND Norbert O. Reich, reich@chem.ucsb.edu.

Two Postdoctoral Research Assistants, University of Durham

Two Postdoctoral Research Assistants, in Theoretical Chemistry and Molecular Physics, to work with Prof. Jeremy M. Hutson University of Durham, England

Applications are invited for two postdoctoral Senior Research Assistantships to work with Prof. Jeremy Hutson on theoretical chemistry and molecular physics. The appointments will be for 1 year in the first instance, starting as soon as convenient (preferably before 1 August 2000). Application may be made either online (via <http://www.dur.ac.uk/Personnel/vacancies/lra.htm> or on forms available from the Personnel Office, University of Durham, Old Shire Hall, Old Elvet, Durham, DH1 3HP (email: Acad.Recruit@durham.ac.uk). Please quote reference A116C. Completed forms, accompanied by a full curriculum vitae and the names of two academic referees, must be received by the Personnel Office by 27 April 2000.

When applying, please make it clear whether you are interested in both of the positions available or just one of them.

The Research Projects and Job Descriptions

Position 1: Long-range forces and cold molecules

It is now possible to trap gas-phase molecules at very low temperatures (below 1 K), and molecule formation in a Bose-Einstein condensate at 10^{-7} K has just been reported for the first time (Wynar et al., Science 287, 1016: February 2000). We have been working on an EPSRC-funded project on long-range interactions between atoms and molecules; the spectra of near-dissociation states of ionic complexes such as He-Ar⁺, Ne-Ne⁺, He-N⁺ and He-H₂⁺, which have been measured by Carrington and coworkers (Southampton), have been used to learn about atomic and molecular interactions at very long range and the dynamics of near-dissociation states (see J. Chem. Phys. 102, 2379 (1995), J. Chem. Phys. 105, 8602 (1996), Chem. Phys. Lett. 260, 395 (1996) and J. Chem. Phys. 110, 3418 (1999) for more details).

The Research Assistant will work Prof. Jeremy Hutson and Dr. Pavel Soldan to understand the role of long-range forces in cold collisions and the properties of cold and ultracold molecules. Interesting questions involve the role of 2-body and 3-body collisions and the behaviour of inelastic and reactive scattering cross sections at very low energies (from 1 K to 10^{-8} K).

Position 2: Fitting potential energy surfaces

We have recently developed a procedure for "morphing" ab initio potential energy surfaces to fit

experimental data. The original potentials need not be of "spectroscopic" quality, but are "bent and stretched" to bring them into agreement with experiment. The morphing procedure offers the prospect of obtaining potentials of "spectroscopic" quality for much larger systems than previously. [See M. Meuwly and J. M. Hutson, "Morphing ab initio potentials: a systematic study of Ne-HF", J. Chem. Phys. 110, 8338-8347 (1999).]

The current project is to extend the morphing procedure in a variety of directions:

Systems involving flexible and vibrating molecules

Systems involving non-linear molecules

Systems involving open-shell atoms and molecules

There may be opportunities for the successful applicants to participate in making research grant proposals and to undertake some teaching duties.

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

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

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

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

Unless otherwise requested before appointment, the Research Assistant will be a member of the Universities Superannuation Scheme, under which the employee's contribution is 6.35% of salary and the University currently contributes an amount equivalent to 12.5%.

Theoretical Chemistry at the University of Durham

Theoretical Chemistry at the University of Durham has been expanding in recent years. There are now four theoretical research groups, which are housed in refurbished space in the newly created Wolfson Centre for Molecular Interactions. The research group leaders are:

Jeremy Hutson: Theoretical chemical physics, especially spectroscopy and dynamics of Van der Waals complexes and clusters; intermolecular forces; molecular collisions; spectroscopic lineshapes and the greenhouse effect.

Mark Wilson: Atomistic simulations of molecular materials, especially liquid crystals.

David Tozer: Fundamental aspects of density-functional theory, especially the development of new functionals that behave properly at long range.

Stuart Althorpe: Chemical reaction dynamics, especially wavepacket methods and their extension to larger reacting systems.

Computers: We have an 8-processor Silicon Graphics Origin 2000 system with 4 GB of shared memory. An additional large multiprocessor machine is currently being purchased.

In addition, the group uses a variety of workstations for program development, and has access to the CRAY T3E supercomputer at Manchester. There is also access to Departmental and central University facilities. All the machines are of course fully networked, with a well-integrated local Ethernet and access to remote sites via SuperJanet.

The Durham/Newcastle Theoretical Atomic & Molecular Physics Group

The Universities of Durham and Newcastle have a very active research community in atomic and molecular physics. The group is interdisciplinary, with members in the Physics and Chemistry Departments at Durham and Newcastle.

The research group leaders outside the Durham Chemistry Department are:

Alan Dickinson (Newcastle Physics): Semiclassical methods for molecular collisions; non-adiabatic processes in atomic collisions; transport and relaxation properties of ions and molecules in gases; collision kernels.

David Flower (Durham Physics): Charge-transfer collisions between atoms; molecular collisions of astrophysical importance.

Ian Cooper (Newcastle Chemistry): Calculation of potential energy surfaces for charge transfer and photoionization applications; use of algebraic methods in molecular spectroscopy, structure and dynamics.
Robert Potvliege (Durham Physics): Multiphoton processes in atoms: theoretical study of multiphoton ionization and of harmonic generation in intense laser fields, laser-assisted scattering processes.
Charles Adams (Durham Physics): Experimental and theoretical studies of laser cooling and atom optics.
Brian Bransden (Durham Physics): Charge-transfer collisions between atoms; positron scattering.
Further information on the Atomic & Molecular Physics group and its activities is available on the World-Wide Web at <http://massey.dur.ac.uk/>

POSTDOCTORAL POSITION, NORTHWESTERN UNIVERSITY

I expect a postdoctoral position to be available in my group as part of the recently established Institute for Environmental Catalysis at Northwestern. The position will focus on studies of a number of reaction processes of critical importance in "real world" environmental problems. One focus is the role of alkyl radicals in lean NO_x chemistry in a zeolite environment. This ties in with other work within the Institute that is directed toward the development of novel catalytic materials that can operate under lean NO_x conditions. Another focus is a detailed understanding of the mechanism(s) of photoinduced reactions of halogenated hydrocarbons on titania (TiO₂) surfaces. This is linked to other studies within the Institute that are directed toward more efficient waste water purification using photo and biocatalytic techniques. Time resolved spectroscopy will be a primary experimental probe in our studies.

This position offers a unique environment for scientific research. A goal of research within the Institute is to use fundamental, molecular level, scientific investigations to address problems in catalysis that bear on "real world" environmental issues. Researchers within the Institute work in a collaborative environment. They come from a number of departments and have a broad range of backgrounds and interests. This environment provides exposure to a variety of perspectives and techniques.

Experience with some aspect(s) of time resolved laser based techniques is desirable. Prior experience with zeolites and/or titania is not a prerequisite. Availability around mid-summer is highly desirable. However, I would consider waiting for an appropriate candidate. An application should include a CV, with publication list, and three letters of recommendation sent to:

Professor Eric Weitz,

Department of Chemistry, Northwestern University

2145 Sheridan Road, Evanston, IL 60208-3113

Phone: 847-491-5583, e-mail : WEITZ@NWU.EDU.

Additional information about the projects and the Institute is available at <http://www.iec.northwestern.edu/> .

Further information about the projects and my reserach interests can also be obtained at

<http://www.chem.nwu.edu/> or by contacting me. Northwestern University is an equal opportunity, affirmative action employer.

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 287 307 (1998), Chem Phys Lett 287 289 (1998), Chem Phys Lett 312 311 (1999), JCP 107 2813 (1997), JCP 110 10269 (1999)); (ii) rate constants (Chem Phys Lett 267 417 (1997), Chem Phys Lett 293 209 (1998)), and (iii) photodissociation cross sections (JCP 105 141 (1996)). Preprints of articles in press (on kinetic energy operators, the discrete variable representation, and a new filter diagonalisation method) are available upon request.

Interested candidates should send a C.V. and a summary of research interests and arrange to have two or three letters of recommendation sent to the address below.

Tucker Carrington Jr., Departement de chimie, Universite de Montreal, Case postale 6128 succursale Centre-ville, Montreal (Quebec) H3C 3J7, Canada
tel: (514) 343-2123, e-mail: Tucker.Carrington@umontreal.ca, fax: (514) 343-7586

EC THEONET - Postdoctoral and predoctoral opportunities

A number of postdoctoral and predoctoral positions are available within the research training network THEONET II (2000 -2004): "Theoretical studies of electronic and dynamical processes in molecules and clusters" funded by the European Commission in the framework of the research and technological development programme "Improving the Human Research Potential and the Socio-economic Knowledge Base" (Fifth Framework Programme of the European Community).

The network is aimed at extending the successes of first-principle computational chemistry, and thereby increasing its impact on and contribution to fundamental and applied chemistry. Some of the research projects are concerned with further theoretical and methodological advances, whilst others address specific chemical problems using new or existing methods.

THEONET II will cover following fields of research

- 1) Quantum Chemistry (molecular electronic structure)
- 2) Potential energy functions, Bound States and Spectroscopy
- 3) Time-dependent Phenomena, Molecular Dynamics and Reactions

Under the terms of the programme, the young researchers who are successful applicants for the supported positions must be aged 35 years or less, and must be nationals of a Community Member State or a State associated with the EC programme (Bulgaria, the Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). Subject to its final conclusion, an Association Agreement signed with the Swiss Confederation is expected to enter into force on 01.01.2001. The young researchers must not be nationals of the state in which the participant appointing them is established, and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

Enquiries should be addressed directly to one of the group leaders of the network:

Prof. P. Rosmus, Theoretical Chemistry, University of Marne la Vallee, Champs sur Marne, F-77454 Marne la Vallee, France; e-mail: p@univ-mlv.fr; phone: +33-160957304; fax: +33-160957320

Prof. P. J. Knowles, School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom; e-mail: p.j.knowles@bham.ac.uk; phone: +44-1214147472; fax: +44-1214147471

Prof. P. Palmieri, Dipartimento Fisica ed Inorganica, University of Bologna, Viale Risorgimento 4, I-40136 Bologna, Italy; e-mail: paolo.palmieri@bo.nettuno.it; phone: +39-0516443698; fax: +39-0516443690

Prof. N. C. Handy, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom; e-mail: nch1@cam.ac.uk; phone: +44-1223336373; fax: +44-1223336362

Prof. G. D. Billing, Chemistry Laboratory III, Department of Chemistry, University of Copenhagen, Univesitetsparken 5, DK-2100 Copenhagen, Denmark; e-mail: gdb@moldyn.ki.ku.dk; phone: +45-35320252; fax: +45-353202591

Prof. L. Halonen, Laboratory of Physical Chemistry, University of Helsinki, P.O. Box 55, FIN-00014 Helsinki, Finland; e-mail: lauri.halonen@helsinki.fi; phone: +358-919140280; fax: +358-919140279

Prof. B. O. Roos, Department of Theoretical Chemistry, Chemical Center, Lund University, P.O.B. 124, S-22100 Lund, Sweden; e-mail: bjorn.roos@teokem.lu.se; phone: +46-46228251; fax: +46-462224543

Prof. G. Delgado-Barrio, Departamento de Fisica Atomica y Molecular Teorica, Instituto de Matematicas y Fisica Fundamental, Consejo Superior de Investigaciones Cientificas, Serrano 123, E-28006 Madrid, Spain; e-mail: gerardo@cc.csic.es; phone: +34-915901607; fax: +34-915854894

Prof. A. van der Avoird, Insitute of Theoretical Chemistry, Chemistry Department, University of Nijmegen, Toernooiveld 1, NL-6525 ED Nijmegen, The Netherlands; e-mail: avda@theochem.kun.nl; phone: +31-243653037; fax: +31-243653041

Prof. V. Aquilanti, Group of Dynamics of Elementary Chemical Processes, General Chemistry Department, University of Perugia, Via Elce di sotto, I-06123 Perugia, Italy; e-mail: aquila@dyb.unipg.it; phone: +39-0755855512; fax: +39-0755855606

Prof. H.-J. Werner, Institut for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany; e-mail: werner@theochem.uni-stuttgart.de; phone: +49 711 685 4400; fax: +49 711 685 4442

Coordinator P. Rosmus

EC REACTIVE INTERMEDIATES - Postdoctoral opportunities

A number of postdoctoral positions are available within the research training network

REACTIVE INTERMEDIATES (2000 -2004): "Laboratory Studies of Reactive Intermediates Relevant to Atmospheric Chemistry and Combustion"

funded by the European Commission in the framework of the research and technological development programme "Improving the Human Research Potential and the Socio-economic Knowledge Base" (Fifth Framework Programme of the European Community).

Scientific co-ordinator: Prof. John M. Dyke, Southampton

Network manager : Prof. Cornelis A. de Lange, Amsterdam

The overall objectives of the REACTIVE INTERMEDIATES network are the development of methods of detection of reactive species in situ; their production in a laboratory environment, to allow further study of their chemistry, and the study of their reactions in the laboratory, in order to allow inferences to be made regarding their reactivity in more complicated systems. In order to allow more focused discussion of the proposed scientific work, the overall objectives have been divided into five key areas:

- 1) Characterisation of Electronically Excited States of Reactive Intermediates
- 2) Spectroscopy of Cations
- 3) Reactive Intermediates Produced by Photolysis and Pyrolysis
- 4) Ion-Molecule Reactions as a Function of Pressure, Temperature and Size
- 5) Heterogeneous Processes on Solid Surfaces and Clusters

An extensive description of the programme can be found on the website for this EEC programme:

http://www.chem.uva.nl/imc/reactive_intermediates.html

Under the terms of the programme, the young researchers who are successful applicants for the supported positions must be aged 35 years or less, and must be nationals of a Community Member State or a State associated with the EC programme (Bulgaria, the Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). Subject to its final conclusion, an Association Agreement signed with the Swiss Confederation is expected to enter into force on 01.01.2001. The young researchers must not be nationals of the state in which the participant appointing them is established, and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

It is expected that the Project will start from September 1st, with postdoctoral appointments being made from that time within the 4 years of the project duration. Each Postdoctoral appointment is for 3 years. Some predoctoral/postgraduate appointments are also available

Enquiries should be addressed directly to one of the group leaders of the network:

Prof. John M. Dyke, Department of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, UK; email jmdyke@pop3.soton.ac.uk; phone +44-1703-593590; fax +44-1703-593781

Prof. Cornelis A. de Lange, Laboratory for Physical Chemistry, University of Amsterdam, Nieuwe Achtergracht 127-129, 1018 WS Amsterdam, The Netherlands; email delange@fys.chem.uva.nl; phone +31-20-5256994; fax +31-20-5256994

Prof. Dolores Guaryacq, Laboratoire de Photophysique Moleculaire, Batiment 210, Universite de Paris-Sud, 91405 Orsay, France; email Dolores.Guaryacq@ppm.u-psud.fr; phone +33-1-69156307; fax +33-1-69156777

Dr. Stelios Couris, FORTH, Institute of Electronic Structure and Laser, PO Box 1527, Vasilika Vouton, 71110 Heraklion, Greece; email couris@iesl.forth.gr; phone +30-81-391470; fax +30-81-391318

Dr. Andy J. Bell, DERA, CB Systems, CBD Porton Down, Salisbury SP4 0JQ, UK; email ajbell@dera.gov.uk; phone +44-1980-613634; fax +44-1980-613834

Prof. Maria de Lourdes Costa, Departamento de Fisica / Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, 2825-114 Monte de Caparica, Portugal; email lurdes@ideafix.df.fct.unl.pt; phone

+351-1-2948576; fax +351-1-2948549

Prof. Vladimir Bondybey, Institute for Physical and Theoretical Chemistry, Technische Universitaet Muenchen, Lichtenbergstrasse 4, Garching, Germany; email bondybey@ch.tum.de; phone +49-89-28913421; fax +49-89-28913416

Dr. Goekhan Baykut, Bruker Daltonik GmbH, Applications Department, Postfach 330126, 28331 Bremen, Germany; email gb@bdal.de; phone +49-421-2205164; fax +49-421-2205101 or +49-421-2205108
March 2000 Cornelis A. de Lange, network manager.

Postdoctoral position, University of Southern California

A postdoctoral position is available in the laboratory of Professor Steve Bradforth in the area of Ultrafast Reaction Dynamics in Solution. The position is immediately available and funded for two years. The candidate should have experience in Ti:Sapphire laser technology, including the maintenance and use of regenerative amplifiers. Experience with optical parametric amplifiers is preferred. Candidates with backgrounds in either gas or condensed phase research will be considered.

Applicants should send a CV by email to bradfort@chem1.usc.edu and arrange for two letters of recommendation to be sent by mail to:

Stephen Bradforth, Department of Chemistry (SSC 702), University of Southern California, Los Angeles, CA 90089-0482, USA

Full details of our reserach program can be found at

http://www-rcf.usc.edu/~bradfort/postdoctoral_announce.html.

For further information please contact bradfort@chem1.usc.edu.

POSTDOCTORAL POSITION AT COMPLUTENSE UNIVERSITY, MADRID

April, 2000

Applications are invited for a postdoctoral fellowship in Gas Phase Reaction Dynamics under the supervision of Professor F. Javier Aoiz and funded by the European Union RTN (Research Training Network) programme, as part of the RTN Network on "Reaction Dynamics: experimental and theoretical studies on the dynamics of reactions of atoms and radicals of fundamental and practical importance". This programme involves seven laboratories: University of Perugia (Italy), University of Oxford (UK), University of Nijmegen (The Netherlands), University of Bielefeld (Germany), University Complutense Madrid (Spain), University of Stuttgart (Germany), University of Muenchen (Germany).

The projects to be developed in our laboratory are concerned with experimental studies of photon initiated elementary chemical reactions in a molecular jet/beam and of photodissociation of molecules containing sulfur and halogens by using resonance enhanced multiphoton ionization (REMPI) and time-of-flight mass spectrometry (TOFMS). In addition, theoretical work based on quasi-classical trajectory and quantum mechanical reactive scattering calculations of the dynamics of the reactions studied experimentally will be performed.

The position (for up to 3 years duration) for young post-doctoral researchers with experimental and/or theoretical skills in the field of Reaction Dynamics is available from April 2000 although the exact commencement date is negotiable. Given the strong links between the different groups in the RTN, the post-doc is expected to spend up to one month each year in another laboratory of the RTN "Reaction Dynamics". Salary is about 3000 euro/month (before taxes). Under the terms of the RTN Programme, the young researcher applicant (aged 35 years or less) must be a national of a Community Member State or a State associated with the RTN Programme (Bulgaria, the Czech Republic, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). The applicants must not be national of the state in which the participant appointing them is established and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to their appointment.

Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcome.

Prof. F. Javier Aoiz, Departamento de Quimica Fisica, Facultad de Quimica, Universidad Complutense,

28040 Madrid, Spain. E-mail: aoiz@legendre.quim.ucm.es; Phone: (+34)91 3944126; Fax: (+34)91 3944135.

Postdoctoral Fellowship, University of Bristol

This position is available as a part of the European Union Research Training Network on Multiply Charged Ions in the Gas-Phase. The proposed starting date is the 1st of July 2000 or as soon thereafter as is mutually convenient. The work will involve:

Ab initio computations on small multiply charged systems, such as the ArC_2^+ or $[\text{CF}_2, \text{H}_2]^{2+}$ systems which are being investigated experimentally in other groups of the network.

The development of global potential energy surfaces for multiply-charged systems, either by interpolation of ab initio computations or by development and parameterisation of semi-empirical models. The range of problems studied here will range from diatomic systems as described above to ion-surface systems.

Chemical dynamics studies of motion on the potential energy surfaces, using classical, semi-classical and quantum-mechanical methods. There will be opportunity to travel to meet other groups in the network. The salary will be towards the lower end of the RAI A scale (e.g. ca. 18,000 per annum), dependent on age and experience. Funding is available for a total of 3 years.

Applicants should have a PhD in either Chemistry or Physics, and an interest in the field of gas-phase ion chemistry and physics. Previous experience in this field, and/or in scientific computing, ab initio computational work, or other areas of chemical physics, would be an advantage. The position is available through the Training and Mobility of Researchers programme of the European Union, and is restricted to nationals of EU countries (as well as some associated countries), excluding the UK.

PhD Studentship

This position is available to EU citizens (including UK!) from October 2000. The subject is relatively free, with the main requirement being that it involves computational or theoretical work relating to a problem in the field of chemical reactivity. Work on any of the areas discussed on the research section of the Group's homepage is obviously possible, as are other projects if mutually convenient. Applicants should hold or expect to hold a first or upper second class degree, or equivalent, in chemistry, chemical physics or physics.

Jeremy Harvey, University of Bristol, School of Chemistry, Cantock's Close, Bristol BS8 1TS

+44 (117) 954 6991 (FAX 925 1295)

Jeremy.Harvey@bristol.ac.uk

<http://www.chm.bris.ac.uk/~chjnh/jeremy.htm>

Postdoc Announcement, Northwestern University

We are looking for a postdoc! The process of dip-pen nanolithography, that was developed by Chad Mirkin at Northwestern, involves preparation of nanostructured patterns on metal surfaces, by deposition from the aqueous meniscus formed between an AFM tip and the metal surface. While this is the macroscopic characterization, there are some wonderful microscopic questions involved: how does the process work? What is the role of surface energy? Does it depend on the speed of deposition or the concentration? What are the forces involved? What are the characteristics of the line, and how does that determine the fractal dimensionality and conductance?

The two of us will be working on this topic together, and we will be delighted to support a postdoc whose interests are in molecular dynamics simulations. If you have somebody with those interests, please let us know. The position will pay a competitive salary, and we think that working in this group on this problem will be challenging and enjoyable.

You can correspond with either of us. Thanks for your help on this and very best wishes.

George Schatz (schatz@chem.nwu.edu)

Mark Ratner (ratner@chem.nwu.edu)

Post-Doctoral Research Assistantship Reaction Dynamics, Oxford University

Applications are invited for a post-doctoral position in the group of Dr Mark Brouard in the Physical and Theoretical Chemistry Laboratory, Oxford University. The research will involve experimental studies of the

stereodynamics of elementary gas phase chemical reactions. Further details of the research activities of the group, and a list of recent publications, can be found at its web page:

<http://physchem.ox.ac.uk/~mb>

The post is tenable for up to three years, subject to satisfactory completion of a six-month probation, and is available immediately. Applicants should preferably have some experience in the use of lasers, and have some background in the field of reaction dynamics. The salary will be on the 1A scale which ranges from 16,286 to 24,479 per annum, depending on age and experience.

The research project is funded by the European Commission, as part of a 4-year Research Training Network (RTN) entitled:

"Reaction dynamics: experimental and theoretical studies on the dynamics of reactions of atoms and radicals of fundamental and practical importance".

Under the terms of the RTN programme, applicants (aged 35 years or less) must be nationals of a Community Member State or a State associated with the RTN programme (Bulgaria, the Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). Applicants cannot be UK nationals, and must not have carried out activities in the UK for more than 12 out of the 24 months prior to appointment.

Applicants should submit a curriculum vitae and arrange for two referees to write directly to Dr M Brouard, The Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ by 14 May 2000.

EMAIL ADDRESS: mark.brouard@chemistry.ox.ac.uk

The University is an Equal Opportunities Employer

Postdoctoral position, University of Arizona

Postdoctoral position, Analytical/Physical Chemist, to work with an interdisciplinary team developing analytical and physical methodology for the detection of molecules of relevance to prebiological chemistry on the surface of Titan. The research effort teams groups at the University of Arizona, Caltech and the Jet Propulsion Laboratory to propose demonstrable schemes for potential future missions to Titan. This position resides in the Departments of Chemistry and Planetary Science, University of Arizona working with Profs. Mark A. Smith and Jonathan Lunine on remote analytical detection of molecules, physical properties of mixtures and the specific detection of enantiomeric excess in laboratory situations matching the surface conditions of Titan. The successful applicant should have experience in at least some of the following areas; manipulation of gases, cryogenics, small scale chromatography (gc and/or hplc), surface adsorption and quartz crystal microbalance techniques. The position is available immediately, however, start dates as late as 9/2000 could be negotiated. The position is anticipated for one year with extensions depending upon mutual consent and funding availability. Please send a cover letter defining interest and availability, vita and the names and full contact information of three qualified references to Mark A. Smith, Department of Chemistry, University of Arizona, Tucson, AZ 85721; or email (msmith@u.arizona.edu) or fax (520 621-8407) The University of Arizona is an EEO/AA employer. Women and minorities are encouraged to apply.

Postdoctoral position, IAMS, Taiwan

Two postdoctoral positions are available immediately in the research group of Dr. Kopin Liu at IAMS, Taiwan. The current experimental programs include (i) developing a novel scheme of coherent control of molecular photodissociation, (ii) molecular photophysics and photochemistry in and on clusters, and (iii) crossed-beam studies of radical reaction dynamics. All projects are fairly challenging and involve a variety of state-of-the-art experimental techniques. Additional information can be glanced at <http://kliu.iams.sinica.edu.tw/>.

We are looking for highly motivated physical chemists or physicists. Experience in laser spectroscopy, vacuum techniques, and computer interfacing of experiments would be preferred, however, the most critical criterion is creativity. The initial appointment will be for one year, with the expectation of renewal for a second year contingent upon reasonable progress. The starting monthly salary is about US\$2,000, and one-way airfare to Taiwan will be reimbursed.

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

to: Dr. Kopin Liu, Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei 10764, Taiwan, Fax: 886-2-2362-0200, email: kpliu@gate.sinica.edu.tw

COMPUTATIONAL SCIENTIST POSITION, Emory University

A position is open for a Ph.D. Computational Scientist in the Cherry L. Emerson Center for Scientific Computation of Emory University. The position will involve:

*Code maintenance and development of molecular modeling programs;

Consult and collaborate with the user community on computational projects;

Prepare documentation, interact with vendors, give short courses on systems, languages and molecular modeling, and maintain peripherals.

Expertise in molecular modeling and familiarity with molecular modeling codes and graphics, as well as good oral and written communication skills, is essential. Also required is familiarity with computer languages such as Fortran and C, C++. The salary will be \$36,000 for 12 months. A small travel budget is also available.

Please submit a CV with publication list and arrange for 2 letters of recommendations to be forwarded to Prof. Keiji Morokuma, Director, Cherry L. Emerson Center for Scientific Computation, Emory University, 1515 Pierce Drive, Atlanta, GA 30322. Review of applications begins on July 1, 2000, and will continue until the position is filled.

Emory University is an affirmative action/equal opportunity employer.

Postdoctoral Position - University of Arizona

Femtosecond Photoelectron Imaging Spectroscopy of Negative Ions

Applications are invited for a postdoctoral position in the laboratory of Andrei Sanov at the University of Arizona. The position is in the area of femtosecond photoelectron imaging spectroscopy of negative ions and ionic clusters. The research focuses on the electronic structure and dynamics of photoinitiated chemical reactions, emphasizing the evolving electronic wave functions. The experimental approach combines the advantages of negative-ion photoelectron spectroscopy, femtosecond pump-probe techniques, and the imaging detection of photoelectrons. The project is in a development stage and the successful candidate will be well positioned to enjoy the benefits of being one of the pioneers in an exciting field.

I am looking for a creative experimentalist who has had experience in some of the following: gas phase reaction dynamics; laser spectroscopy; photoelectron or photofragment spectroscopy; photoelectron or photofragment imaging; mass-spectrometry; femtosecond lasers; high vacuum systems.

The position is available starting in July or August 2000, although a later starting date could be negotiated.

The initial appointment will be for one year with the expectation of extensions contingent upon reasonable progress and funding availability. The compensation package will be competitive, commensurate with qualifications. Tucson, Arizona is a great yet inexpensive place to live, with excellent climate and breathtaking scenery, world-class hiking, rock climbing, mountain biking, and even skiing.

Interested candidates should send a curriculum vita, a full list of publications, a brief summary of previous research experience, and the names and full contact information of three qualified references willing to write letters of recommendation to Prof. Andrei Sanov, Department of Chemistry, University of Arizona, Tucson, AZ 85721-0041, U.S.A. Alternatively, the application materials can be sent by e-mail (sanov@u.arizona.edu) or fax (520 621-8407).

Postdoctoral positions in single molecule spectroscopy

Two postdoctoral positions are immediately available under the supervision of Dr David Klenerman and Dr Shankar Balasubramanian in the Department of Chemistry, Cambridge University. These positions are for one year in the first instance. The project is to study single fluorophor labeled biomolecules attached to surfaces using total internal reflection fluorescence spectroscopy with an ICCD detector and to perform enzymatic reactions on these molecules, probed by changes in fluorescence. This project is sponsored by a local company with the possibility of full time employment at the end of the project. We are looking for someone with experience in fluorescence spectroscopy, image analysis or the surface attachment of biological molecules. To apply please send a CV and the name of two referees to:

Dr David Klenerman, Department of Chemistry, Cambridge University, Lensfield road , Cambridge CB2 1EW

Fax : 01223-336362 Email dk10012@cam.ac.uk

Postdoctoral position

I have postdoctoral openings in two areas:

1) Spectroscopic studies of urban particulate matter 2) Satellite and laboratory studies of stratospheric clouds and aerosols.

Professor James Sloan, Departments of Chemistry and Physics, University of Waterloo, Waterloo ON N2L 3G1, CANADA

<http://www.sciborg.uwaterloo.ca/~sloanj>

<http://www.sciborg.uwaterloo.ca/wcas>

Tel: +1 519 888 4401, Fax: +1 519 746 0435, e-mail: sloanj@UWaterloo.CA

POSTDOCTORAL RESEARCH POSITION IN ATMOSPHERIC OXIDATION PROCESSES PORTLAND STATE UNIVERSITY

A postdoctoral research position is available in the Atmospheric Chemistry Research Group associated with the Chemistry Department at Portland State University in Portland, Oregon. The position will begin October 1, 2000. The project will involve a novel use of atmospheric pressure ionization mass spectrometry for the direct investigation of complex atmospheric oxidation mechanisms of hydrocarbons. A suitable candidate will have an interest in the application of modern physical methods to the study of atmospheric chemical processes.

Candidates with a recent Ph.D. and a background in experimental physical or analytical chemistry or atmospheric chemistry, and research experience in applications of mass spectrometry to atmospheric and/or chemical reaction kinetics should send their curriculum vitae and three letters of reference to Professor Robert J. O'Brien at the address below. The position is initially for one year but is renewable.

Interested candidates should write to; Professor Robert J. O'Brien, Department of Chemistry, Portland State University, 1719 SW 10th Ave SB2-262, Portland, OR 97201

Email: obrienr@pdx.edu, Tel: (503) 725-4264, Fax: (503) 725-3888

POSTDOCTORAL RESEARCH POSITION, JAIST, Japan

A postdoctoral research position involving collaborative research among a few groups in physics and chemistry at JAIST (Japan Advanced Institute of Science and Technology) is available. JAIST is a new (established 7 years ago) research and educational institution established by the Japanese Ministry of Education for graduate studies. The research involves fundamental exploration of condensed matter and biological systems. Recent developments at our lab in femtosecond visible and IR time-resolved spectroscopy will be used to observe directly the dynamic response of materials undergoing sudden optical excitation. The research involves 1) femtosecond pump-probe analysis of photoexcited carrier lifetimes and excitonic nonlinear effects in various GaAs epilayers and GaAs/AlAs multiple quantum well structures which are grown by molecular beam epitaxy at low temperatures. 2) Primary energy and electron transfer processes in plant photosynthesis, particularly photosystem 1 reaction center, 3) Primary processes in gene signal generation etc. The position is for one year with one additional year possible based on first-year progress. Experience in femtosecond time-resolved spectroscopy strongly preferred. Applicants should have a CV and at least three letters of recommendation sent to the address below.

Prof. Keitaro Yoshihara, School of Materials Science, JAIST, Tatsunokuchi 923-1292, JAPAN
yosihara@jaist.ac.jp

Postdoctoral Position in Theoretical/Computational Chemistry, University of Michigan

Applications are invited for a postdoctoral position in the newly established research group of Professor Eitan Geva at the University of Michigan. I am looking for a person with a strong theoretical/computational background, who has interest in one of the following research projects:

(1) Computational solution-phase quantum and semi-classical dynamics.

(2) Theory of single molecule spectroscopy in biomolecules.

(3) Theory of spectroscopy in glasses.

(For more details see www.umich.edu/~michchem/faculty/geva/).

The position is available starting in October 2000. The initial appointment will be for one year, with the expectation of extensions contingent upon reasonable progress. The compensation package will be competitive, commensurate with qualifications. Ann Arbor is a vibrant and cosmopolitan University town, that offers a high standard of living, diverse cultural atmosphere, and numerous opportunities for outdoor activities.

Interested candidates should send a curriculum vita, a full list of publications, a brief summary of previous research experience, and three reference letters, to:

Until August 1 2000:

Dr. Eitan Geva, Department of Chemistry, University of Utah, 315 S. 1400 E., Salt Lake City, UT 84112
801-581-8606 (W), 801-581-4353 (FAX)

Eitan.Geva@hec.utah.edu

After August 1 2000:

Professor Eitan Geva, Department of Chemistry, University of Michigan, 930 N. University, Ann Arbor, MI
48109-1055

eitan@umich.edu

Postdoctoral position, Emory University

A POSTDOCTORAL POSITION is available to investigate predissociation and intermolecular reaction dynamics of open shell van der Waals complexes. Experiments involve process initiation via electronic excitation or stimulated Raman pumping. Products are characterized using LIF, REMPI, and HRTOF techniques. Candidates should have a Ph. D. in experimental physical chemistry with previous experience in laser spectroscopy. Send resume and three letters of recommendation to Prof. Michael C. Heaven, Department of Chemistry, Emory University, Atlanta, GA 30322.

POSTDOCTORAL POSITION, Hebrew University

Quantum Chemistry method development, Prof. Roi Baer, The Hebrew University of Jerusalem

The group of Prof. Roi Baer at the Hebrew University of Jerusalem Israel has a post-doctoral position opening for physicists and theoretically oriented chemists interested in research involving the development of computer methods for calculations of the electronic structure of large molecules.

This project is part of a collaboration with the UC Berkeley group headed by Prof. Martin Head-Gordon.

Research topics include developing linear scaling ab initio density functional methods to be implemented on large molecular systems. Candidates should have a general familiarity with computational methods and programming Techniques in FORTRAN and C++.

Details on topics of Prof. Baer and Head-Gordon's research are available at

<http://www.fh.huji.ac.il/~roib> <http://www.cchem.berkeley.edu/~mhgrp>

Interested candidates should send a resume, statement of research interests, unpublished preprints, and three letters of recommendations to Prof. Baer at the addresses below.

Roi Baer, Dept. of Physical Chemistry and the Lise Meitner, Center for Quantum Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Tel: 972-2-658-6114 Fax: 972-2-651-3742

email: roib@fh.huji.ac.il, Web: <http://www.fh.huji.ac.il/~roib>

Two postdoctoral positions in the University of Helsinki, Finland

Two postdoctoral positions funded by the European Community are available in the Laboratory of Physical Chemistry for about two years starting August 2000. The monthly salaries are about 2520 Euro. One of the successful candidates is expected to carry out experimental research in the field of laser spectroscopy, particularly developing new spectroscopic laser methods for molecular overtone state studies. The other position is in the field of theoretical and computational molecular spectroscopy, particularly developing new Hamiltonian models for highly excited vibrational states including large amplitude problems. Experience in

electronic structure calculations is also welcome. For some of our publications in the experimental spectroscopy see J. Chem. Phys. 110, 1424 (1999); 107, 1680 (1997); 104, 488 (1996); 102, 3911 (1995); 99, 3277 (1993); Rev. Scient. Instr. 63, 5546 (1992); Chem. Phys. Letters 189, 205 (1992) and in the theoretical spectroscopy see Adv. Chem. Phys. 104, 41 (1998); J. Chem. Phys. 112, 3121 (2000); 111, 3018 (1999); 110, 7339 (1999); 106, 831 (1997); 102, 3945 (1995). The Helsinki molecular spectroscopy group has excellent experimental and computational facilities. The group consists of about 10 people. Under the terms of the EC programme, the young postdoctoral researchers, who are successful applicants for the supported positions, must be aged 35 years or less, and must be nationals of a Community Member State or a State associated with the EC programme (Bulgaria, the Czech Republic, the Republic of Cyprus, Estonia, Hungary, Iceland, Israel, Latvia, Liechtenstein, Lithuania, Norway, Poland, Romania, Slovakia and Slovenia). Subject to its final conclusion, an Association Agreement signed with the Swiss Confederation is expected to enter into force on 01.01.2001. The young researchers cannot be nationals of Finland. More information can be obtained from Prof. Lauri Halonen, tel. +1-303-492-8046, fax +1-303-492-5235, e-mail lauri.halonen@helsinki.fi, home page <http://fkassistant.pc.helsinki.fi/>
Please send the applications to the address: Prof. Lauri Halonen, JILA, University of Colorado at Boulder, Campus Box 440, Boulder, Colorado 80309-0440, USA. The closing date is 22nd June 2000.

Postdoc Positions in European Research Network COCOMO

We offer postdocs positions in experimental and theoretical physics (or physical chemistry) in one of the research groups in GERMANY, UNITED KINGDOM, ISRAEL, GREECE, THE NETHERLANDS, SWEDEN, BULGARIA, or FRANCE. Those groups form the COCOMO-Network ("Coherence and Control in Atomic and Molecular Systems and Processes") which was selected for funding by the European Union and started its operation on March 1, 2000.

We investigate new ways for the control of atomic and molecular systems and processes by light-matter interaction. The COCOMO partners are well established groups with international reputation working in the field of laser-based manipulation of atoms and molecules, e.g. laser-based control of chemical reactions, development of new radiation sources, laser physics, nonlinear optics, high-intensity light-matter interactions, investigation of ultra-fast processes, theoretical and experimental quantum optics and chemical physics and much more! The laboratories are equipped with edge-of-technology laser systems, permitting research at one of the frontiers of today's laser-based physics and chemistry. The theoretical groups are equipped with powerful work stations and computers.

Postdoc positions are available in the research groups at University of Kaiserslautern, Germany (network coordinator) (K.Bergmann, T.Halfmann);

Imperial College, London, UK (P.L.Knight, J.Marangos);

FORTH, Heraklion, Greece (D.Charalambidis, P.Lambropoulos);

University of Wuerzburg, Germany (G.Gerber);

The Weizmann Institute, Rehovot, Israel (M.Shaipro);

The Royal Institute of Technology, Stockholm, Sweden (S.Stenholm);

FOM, Amsterdam, The Netherlands (L.D.Noordam);

Paul Sabatier University, Toulouse, France (B.Girard);

Bulgarian Academy of Sciences, Sofia, Bulgaria (N.Vitanov).

We offer the possibility for challenging and fascinating work both in experimental and theoretical physics. Candidates should have some experience with at least one of the research topics mentioned above and be motivated to work successfully in a dynamic environment with lots of international contacts and visitors.

The salaries are attractive, based on European standards. Only citizens of the European Union or associated countries (Israel, the Baltic States, Bulgaria, Romania, Poland, Hungary, Czech Republic) can be appointed. The host laboratory must not be located in the country of citizenship of the candidate.

For further detailed information contact us NOW !

email : halfmann@physik.uni-kl.de

website : <http://www.cocomo-network.de>

RESEARCH FELLOW, UNIVERSITY OF ABERDEEN

16,286 - 18,185 pounds per annum

Required to work within the Department of Chemistry with Dr. Mark Law on theoretical chemistry and molecular physics. The project which is ESPRC funded will involve regular and close consultation and interaction with Prof. Jeremy M. Hutson (Durham) and Prof. Jonathan Tennyson (University College London). Funding is available for up to 3 years, starting on 1 September 2000. The Research Fellow will work on the development of methods and general-purpose computer programs adapted to the challenging problem of accurate calculation of rotation-vibration quantum state energies and wavefunctions of tetraatomic molecules exhibiting wide-amplitude motion. Applications will include the spectroscopy and bonding of chemically bound and Van der Waals systems. Applicants should have a PhD in a relevant area with a good background in spectroscopy, theoretical chemistry, chemical physics or scattering theory, and should be interested in and talented at computational work.

Informal enquiries may be directed to Dr Mark M. Law, Department of Chemistry, telephone 01224 272933 (UK) or +44 1224 272933 (International) or e-mail m.m.law@abdn.ac.uk.

Application forms and further particulars are available from Human Resources, University Office, University of Aberdeen, King's College, Aberdeen AB24 3FX, telephone 01224 272727 (UK) or +44 1224 272727 (International) or e-mail personnel@abdn.ac.uk. Please quote reference number YCM008R

Completed forms, accompanied by a full curriculum vitae and the names of three academic referees, must be received by the Human Resources Office by 16 June 2000.

An Equal Opportunities Employer

Further Particulars

Aberdeen University reference number YCM008R

The Research Project and Job Description

Rovibrational Quantum States of 4-atom systems: Recent advances in experimental spectroscopy and the requirements of atmospheric chemistry, astrophysics and combustion chemistry have led to a need for the accurate prediction and understanding of the high lying (wide-amplitude) vibration-rotation states of small molecules. Great progress has recently been made in the variational calculation of the vibration-rotation energy levels, wavefunctions and spectroscopic transition intensities of triatomic molecules and such calculations are now becoming routine (for closed-shell systems). However high precision rotation-vibration calculations on tetraatomic species represent an important frontier in the quantum molecular dynamics field. Systems involving multiple minima and/or high rotational excitation are particularly challenging and represent the major targets of this project.

The Research Fellow will work with Dr. Mark Law to produce a suite of computer codes usable by a wide research community and capable of accurate calculations of the rovibrational bound state energies and wavefunctions (and hence transition intensities) of all closed-shell tetraatomic molecules and complexes.

The computer programs will be developed using Sun and Dec-Alpha workstations in Aberdeen, with access to the Cray T3E parallel supercomputer facility at Manchester (CSAR) for computationally intensive work.

There is also access to Departmental and central University facilities. All the machines are of course fully networked, with a well-integrated local Ethernet and access to remote sites via SuperJanet.

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

Although based in Aberdeen, the Research Fellow will be expected to collaborate with other groups in the UK, to ensure that the programs developed are useful to the CCP6 community as a whole (see below). In particular the project will involve regular and close consultation and interaction with Prof. Jeremy M. Hutson (Durham) and Prof. Jonathan Tennyson (University College London).

In addition to this research work, the Research Fellow will take a role in coordinating CCP6 activities and helping to organise CCP6 Working Group meetings and conferences.

Interests of Research Groups Associated with the Project

Dr. Mark Law (Aberdeen): Theoretical interpretation of molecular spectra; vibration-rotation energy levels of small molecules; intramolecular vibrational energy redistribution; determination of molecular potential

energy surfaces; computational chemistry using parallel computing methods; development of the methodology of fitting physical models to data.

Further information on Mark Law's research group and the University of Aberdeen is available at <http://www.abdn.ac.uk/~che194/>

Prof. Jeremy Hutson (Durham): Theoretical chemical physics, especially: spectroscopy and dynamics of Van der Waals complexes and clusters; intermolecular forces; molecular collisions; spectroscopic lineshapes and the greenhouse effect.

Further information on Jeremy Hutson's research group is available at <http://www.dur.ac.uk/~dch0www/Staff/jmh/jmh.group.html>

Prof. Jonathan Tennyson (University College London): Theoretical atomic and molecular physics and astrophysics, including: spectroscopy and collisions of atoms and molecules, fundamental classical and quantum dynamics, the calculation of atomic and molecular data for astrophysics, and modelling of both spectra and atmospheres.

Further information on Jonathan Tennyson's research group is available at <http://www.tampa.phys.ucl.ac.uk/jonny/>

The CCP6 Consortium

The Collaborative Computational Project on Heavy Particle Dynamics comprises 18 research groups who work together to maintain the United Kingdom's high international standing in the field of molecular quantum dynamics. CCP6 has developed considerable expertise in the effective use of (massively) parallel computers, a vital contributing factor to the consortium's considerable scientific impact over the last 25 years. Further information on CCP6 and its activities is available at <http://www.cse.clrc.ac.uk/Activity/CCP6>

The City of Aberdeen (also known as the "Silver City" or the "Granite City") is a medium size, historic University city in the north-east of Scotland. In addition to the University, its attractions include a rich cultural (including architectural) heritage, a strong local economy, and easy access to attractive coastlines and lowland and highland areas which offer superb opportunities for (hill)walking and skiing.

Further information on the City of Aberdeen is available at <http://www.abdn.ac.uk/central/abdn/index.htm>

OPEN POSTDOCTORAL POSITION, CHEMICAL PHYSICS THEORY, GROUP PROFESSOR PAUL BRUMER, UNIVERSITY OF TORONTO

Postdoctoral applicants are sought for a position in theoretical chemical physics, either in the study of coherent control of molecular processes or in semiclassical mechanics. A background in theoretical or computational Chemistry or Physics is required. Previous experience in either semiclassical mechanics or in the study of light interacting with matter would be a great asset.

Interested applicants should write Paul Brumer at pbrumer@tikva.chem.utoronto.ca or at

Prof. Paul Brumer, Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 3H6

Postdoctoral Openings, Air Force REsearch Laboratory

Up to two National Research Council Associate positions are available at the Air Force Research Laboratory at Hanscom Air Force Base, 15 miles northwest of Boston, Massachusetts. We perform laboratory research to better understand the chemistry and physics of the upper atmosphere. The research is conducted in an academic style and results are published in the open literature. U.S. citizenship is required for these positions, and applicants should be either soon-to-be or recent (past five years) PhD's.

A modest-length proposal, written with input from an AFRL staff member, is due 15 Aug 2000 together with supporting documents. The position is nominally for one year, although it is typically extended to two years contingent on mutual agreement. Salary is about \$45,000/year.

See "<http://national-academies.org/rap> for further details. We encourage submissions from motivated individuals, including those who wish to broaden their experimental knowledge base. Please contact the appropriate scientist (see below) for further information.

Position 1: Experiments in the COCHISE (COLD CHEMical Infrared Simulation Experiment) facility will be

pursued, specifically the spectroscopy and kinetics of excited nitrogen atom collisions with oxygen molecules [$\text{fast N} + \text{O}_2 \rightarrow \text{NO}(v, \text{high } J) + \text{O}$]. The details of the very highly rotationally excited product states of NO will be investigated as a function of precursor state. Metastable species will be monitored using spectrometric and interferometric detection of visible and IR emissions. Please contact Dr. Steve Miller at 781.377.2807 or Steven.Miller@hanscom.af.mil for further information.

Position 2: Experiments in the laser laboratory investigating energy transfer in key aeronomic processes will be pursued. Notably, these include vibrational energy transfer in collisions of NO and CO₂ with oxygen atoms. Techniques such as laser-induced fluorescence, transient diode laser absorption, and time-resolved Michelson interferometry will be used to detect the relevant species. Complex spectral and kinetic models will be developed to analyze and interpret the resultant data. Please contact Dr. Jim Dodd at 781.377.4190 or James.Dodd@hanscom.af.mil for further information.

POSTDOCTORAL POSITION, C. S. PARMENTER RESEARCH GROUP, INDIANA UNIVERSITY

A postdoc appointment for a recent PhD is available with the experimental chemical physics group of C. S. Parmenter. The research concerns vibrational and rotational dynamics in gas phase molecules with six to thirty modes.

Two studies focusing on collisional energy transfer will receive much attention in the next few years. One is designed to reveal the steric effects that underlie these collisional interactions. While predicted by theory to be large, steric influences on inelastic collisions with polyatomics have never before been experimentally accessible. We are using crossed molecular beams to give state-to-state resolution of single collision rotational and rovibrational energy transfer channels in planar or near-planar symmetric top molecules. A laser pumps an initial vibrational level in an electronically excited state with selected angular momentum around the top axis. To achieve control over the collision geometry, molecules are aligned using the laser polarization as guided by recent theory. (JCP 107, 7138 (1997), JPC-A 101, 9594 (1997)) The alignment establishes bias toward edge-on or broadside encounters. Dispersed fluorescence yields relative cross sections for the competition among dozens of individual rotational and rovibrational channels that will produce a comprehensive picture of steric influences.

The other is directed at the collisional activation/deactivation of large molecules with the high vibrational energy needed for unimolecular reaction. Despite years of study, one basic measurement remains elusive, namely the absolute total cross section for energy transfer into the neighboring vibrational field for these highly excited molecules. We are using a new twist on our oxygen fluorescence quenching method (chemical timing) that has long been associated with collision-free vibrational dynamics to produce these measurements. The method is adapted to a collisional environment that produces absolute cross sections for vibrationally excited molecules with state densities of thousands of levels per wave number.

Applicants should submit a CV and arrange to have letters of recommendation sent on their behalf.

Prof. Charles S. Parmenter, Department of Chemistry, Indiana University, Bloomington, IN 47405, USA
Email: parment@indiana.edu, Office: (812) 855-3522, Fax: (812) 855-8300

POST-DOCTORAL POSITION AT EPA

Chemical Physicist/Physical Chemist with experience in the use of laser-based spectroscopic methods for measurement of gaseous species. The ideal candidate will have hands-on experience with resonance enhanced multiphoton ionization (REMPI) or other laser spectroscopy of molecules. The candidate will work in an applied program that couples REMPI with time-of-flight mass spectrometry (TOFMS). The candidate will work with the leading international laser spectroscopy groups developing the REMPI analytical method and designing and building an instrument for use at EPA. Candidate will apply REMPI instrument for detection of trace halogenated air toxics as part of a comprehensive program at the EPA's combustion research facility in Research Triangle Park, NC, investigating the formation mechanisms of these pollutants.

Background

The U.S. EPA's Office of Research and Development, National Risk Management Research Laboratory (Research Triangle Park, NC) conducts research on formation mechanisms, quantification methods, and prevention of hazardous air pollutants, particularly halogenated organics such as chlorinated

dibenzodioxins/dibenzofurans, biphenyls, and naphthalenes. Recently, NRMRL has been awarded a grant to study the application of REMPI/TOFMS techniques toward development of a real time "dioxin" monitor. This grant program, combined with a DOE-funded program to develop the instrumental science behind REMPI/TOFMS, constitutes a large federally-funded effort whose goal is to develop this method of hazardous air pollutant detection for source characterization, understanding of pollutant formation mechanisms, and pollution prevention. As part of this program, a REMPI/TOFMS system will be built for use at EPA's combustion research facility. The post-doctoral laser spectroscopist is necessary to operate the REMPI/TOFMS system and develop its application for trace halogenated species detection. Candidate will work with a team of researchers investigating hazardous air pollutant formation on in-house facilities including waste combustors, industrial boilers, solid fuel combustors, rotary kilns, and laboratory reactors.

Particulars
The optimal timing for arrival of this post-doctoral candidate is January-March, 2000. This timing will allow the candidate to work with the REMPI developer as they put together the instrument, allowing the candidate to better understand how the REMPI/TOFMS system works. Salary is US\$48,000 per year. This position is open to foreign nationals as well as U.S. citizens.

Information

Further information can be obtained by contacting Dr. Brian Gullett, (919)541-1534, gullett.brian@epa.gov

Post-Doctoral Research Assistant University of Bristol, UK

'SiO Maser Modelling - Assessment of Mass Loss and Hydrogen Concentrations in Late Type Stars'
Applications are invited for a post-doctoral position to work on a challenging project which seeks to investigate the rate of mass-loss from late type stars.

The candidate should have expertise in one or more of the following areas: 1) quantum-mechanical scattering theory; 2) ab-initio molecular electronic structure theory; 3) radiation transport and hydrodynamics. The project will use advanced techniques and computer codes from all these disciplines at different stages.

The objectives of the project will be to model the SiO maser radiation from the region of late type stars and from this modelling to ascertain the state and quantity of the hydrogen gas present in the region where mass-loss is initiated. This in turn will permit an estimation of the rate of mass loss from the stars involved. In order to model the maser radiation an improved knowledge of the vibrationally-rotationally inelastic collision cross sections of SiO with the most abundant available collision partners is needed. The project is already well under way and we have nearly finished the calculation of the necessary interaction potentials. The next stage of the project will be the computation of inelastic collision cross sections using these potentials followed by the use of the computed cross sections in maser modelling calculations.

The successful candidate will work with Prof. Gabriel Balint-Kurti (School of Chemistry), Dr. Malcolm Gray (Department of Physics and Astronomy, University of Wales, Cardiff) and Prof. David Field (Institute of Physics and Astronomy, Aarhus, Denmark). Applications should be made to Prof. G.G. Balint-Kurti (School of Chemistry, University of Bristol, Bristol BS8 1TS, UK) and should supply the names of two referees.

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

POSTDOCTORAL FELLOWSHIPS IN ELECTRON and LASER SPECTROSCOPY IN THE DEPT. OF CHEMISTRY , SOUTHAMPTON UNIVERSITY

Applications are invited for two postdoctoral fellowships, each to work for up to 3 years ,in the research group of Professor John Dyke.

Applicants should have a Ph.D in Chemistry or Physics.Experience in electron spectroscopy,molecular spectroscopy,vacuum technology or laser technology would be an advantage ,but is not essential. The first position is available from January 1st 2000,whilst the second position is available from September 1st 2000. The first post involves the study of reactive intermediates using photoelectron spectroscopy with synchrotron radiation,and electron scattering, while the second position involves the study of radicals and

molecular complexes with laser multiphoton ionization and related techniques.
Informal enquiries should be directed to Prof John Dyke at jmdyke@soton.ac.uk,
or see <http://www.soton.ac.uk/~physchem.htm>

Postdoctoral Research Position, University of Pittsburgh

A Surface Probe Microscopy (STM/AFM) postdoctoral position is available in the Solid/Liquid Interface Group of the Surface Science Center at the University of Pittsburgh. The project is focused on the study of interface dynamics at the atomic and molecular level. Candidates should have previous experience with STM/AFM, especially in electrochemical environments. Experience with lasers and optics is a plus. The candidate should have strong problem solving skills, work well with others and demonstrate scientific leadership and initiative. As we also have Second Harmonic and Sum Frequency projects ongoing, this position is an excellent opportunity to learn more about linear and non linear optical probes of interfaces. The Surface Science Center at the University of Pittsburgh provides an excellent research environment. 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. Pittsburgh is safe, pleasant and affordable city offering the amenities of a major metropolitan area. 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.

Applications should be sent to: Dr. Eric BORGUET, Department of Chemistry and Surface Science Center, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh PA 15260, U.S.A.

(412) 624-8304 Office, (412) 624-8611 Fax

borguet+@pitt.edu, <http://www.pitt.edu/~borguet/>

Postdoctoral Position, Concordia University, Quebec

Post-Doctoral or Graduate Ph.D. Assistantship is available immediately in Theoretical/Computational (and possibly Experimental) Biochemistry. We are seeking outstanding candidates to investigate the role of proton transfer and hydrogen bonding in enzymatic reactions, as part of an international collaboration between various theoretical and experimental research groups at Concordia University and in France. The successful candidate will conduct theoretical research with Prof. Gilles H. Peslherbe (Concordia University, Montral, Canada) and with Dr. James T. Hynes (at Ecole Normale Suprieure, Paris, France), primarily in connection with experiments performed at Concordia University in Prof. Ann English Laboratory. He/she may also have the opportunity to perform experimental research with Prof. Ann English. Applicants must be eligible for a Chateaubriand fellowship, which provides generous funding for studying one year in France. Interested and qualified candidates should contact Dr. Peslherbe immediately and/or send a complete Graduate School application to the Department of Chemistry and Biochemistry, Concordia University, 1455 De Maisonneuve Blvd West, Montral, Qubec, CANADA H3G 1M8. Fax: (514) 848-2868. E-Mail: ghp@alcor.concordia.ca. For more information, see <http://artsci-ccwin.concordia.ca/facstaff/p-r/peslherbe>

Institute of Atomic and Molecular Sciences, Academia Sinica Department of Physics, National Taiwan University

Positions are open for POSTDOCS with Yuan T. Lee and Ralf I. Kaiser in the Institute of Atomic and Molecular Sciences (Academia Sinica) and the Department of Physics (National Taiwan University). We employ cutting edge crossed beams and matrix isolation techniques in the fields of material sciences, catalyses, combustion chemistry, and physical processes in interstellar environments and our solar system. The following research topics are available:

1. Formation and properties of boron and silicon bearing molecules relevant to semiconductor industry
2. Elementary mechanisms in 3d-group transition metal or zeolite catalyzed reactions (e.g. ices condensed on Fe, Ni, and Co layers)
3. Reaction dynamics in elementary processes in chemical vapor deposition (CVD) of carbon, boron, and silicon containing molecules

4. Formation of polycyclic aromatic hydrocarbon (PAH) molecules and soot in combustion processes and extraterrestrial environments
5. Synthesis of molecules in the gas phase or icy bodies in the interstellar medium or our solar system such as Jupiter, Saturn, Uranus, Neptune, Pluto, and especially Titan.
6. Synthesis of unstable radical intermediates in organic and metallo organic chemistry.
7. Formation of precursor molecules on proto Earth and extraterrestrial environments to biomolecules like carbon hydrates, DNA, and aminoacids.

Outstanding candidates with a high research commitment should send inquiries to Dr. Ralf I. Kaiser, Institute of Atomic and Molecular Sciences, Academia Sinica, 1 Section 4, Roosevelt Rd., Taipei, 106, Taiwan, ROC. Tel: 886-2-23645370; Fax: 886-2-23620200; email: kaiser@po.iam.s.sinica.edu.tw.

Postdoctoral position, Department of Chemistry, Cambridge University

A postdoctoral position is available immediately for three years to develop a new method to image channels and receptors on living cells. The method is a novel combination of scanning ion conductance microscopy (see for example *Biophys. J.* 73,653-658 (1997)) with fluorescence microscopy. This is joint project between Dr David Klenerman (Department of Chemistry, Cambridge University) and Dr Yuri Korchev (Department of Medicine, Imperial College, London). A good experimental background in scanning probe microscopy or fluorescence methods would be desirable but no prior knowledge of cell biology is required. To apply please send a copy of a curriculum vitae and the names of three referees to :

Dr David Klenerman, Dept Chemistry, Cambridge University, Lensfield Road, Cambridge CB2 1EW
Email dk10012@cam.ac.uk Tel: 44-(0)1223-336481 Fax: 44-(0)1223-336362

or

Dr Yuri Korchev, Imperial College School of Medicine, Division of Medicine, 5th floor MRC Clinical Sciences Centre, Hammersmith Campus, Du Cane Road, London W12 0NN
Email: y.korchev@ic.ac.uk Tel.: 44(0)181 383 2362 Fax: 44(0)181 383 8306

Postdoctoral Position in Environmental Chemistry at SRI International

The Molecular Physics Laboratory at SRI International has been awarded a Postdoctoral Fellowship by the Camille and Henry Dreyfus Foundation to employ a Ph.D. Chemist or Chemical Engineer to perform laboratory research in atmospheric chemistry.

Current research directions in our laboratory include experimental studies using Knudsen cell techniques and an aerosol flow reactor to address issues of stratospheric and tropospheric relevance. Choice of research topic will depend on the skills and interests of the postdoctoral scientist. Some areas of potential research are: heterogeneous chemistry on sulfuric acid surfaces heterogeneous chemistry on soot and/or mineral dust particles effect of trace metals in atmospheric particles role of iron catalysis in the reactions of organics in cloud and rainwater fate of biogenic emissions aqueous phase formation of multifunctional carboxylic acids The postdoctoral researcher will play a large role in the development of some of the above activities.

Familiarity with vacuum techniques and mass spectrometry is desirable, as is experience with spectroscopy, chromatography, LabView programming, or chemical synthesis. The successful candidate will be chosen based on her/his chemical talents and commitment to environmental studies but is not expected to have prior training in atmospheric chemistry. Salary is competitive, and the Fellowship is renewable for a second year by mutual agreement of the Fellow, research supervisors, and the Dreyfus Foundation. Applications, including a curriculum vitae, selected publications and/or thesis abstract, statement of specific research interests, and at least two letters of recommendation should be sent to: David M. Golden or Laura T. Iraci, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave, Menlo Park, CA 94025. e-mail: golden@sri.com or laura.iraci@sri.com. (<http://www.sri.com/jobs/listings/32077.html>) Candidates are encouraged to apply by February 29, and review will continue until the position is filled.

Postdoctoral Positions, The Royal Institute of Technology, KTH, Stockholm

The Goran Gustafsson POSTDOCTORAL FELLOWSHIP The Departments of Physics, Mathematics and Mechanics at the Royal Institute of Technology (KTH), Stockholm, Sweden, invites applications for one or two postdoctoral fellowships.

The successful candidate is expected to join an existing research group at one of the departments (mathematical, mechanics or physics) at the School. The duration of the stay is a minimum of 9 months and a maximum of 12 months, preferably beginning during the summer of 2000.

Candidates should submit, so as to arrive at KTH before March 1, 2000 a Curriculum Vitae (maximum 2 pages) and a list of publications, two or three letters of recommendation, including one from the research group of interest and a description of what work the candidate plans to perform at KTH (maximum 1 page). (Candidates cannot have their PhD degree from KTH or the Stockholm area.)

The stay at KTH must begin before September 1, 2000.

Applications should be sent to:

Utbildningskansli DEF, KTH, S-100 44 STOCKHOLM, SWEDEN

Questions are preferably sent to any contact person you may have at the Departments of Mathematics, Mechanics or Physics. Please note reference number: 200-09-00

Information can also be found on the web: <http://www.atom.kth.se/~berg/pdoc.html>

Postdoctoral Position, Loughborough University

A one year postdoctoral position is available, starting immediately, for 1 year on a European framework 5 project entitled "Study for the construction of a Quantum Information Processing Device using Doped Fullerenes". The work will involve using both classical dynamics and quantum (LDA) calculations on the structures of various doped fullerenes and their energetic interactions with different surfaces. Candidates should hold a Ph.D. or have equivalent research experience and have good computing and physical modelling skills. The salary will be 21,134 per annum for a start date of 1 March 1999.

Further information can be obtained from Professor Roger Smith, School of Mathematics and Physics, Loughborough University, Leicestershire, LE11 3TU, UK. (email: R.Smith@lboro.ac.uk)

Postdoctoral Position, University of Birmingham

Applications are invited for a postdoctoral fellowship on a project in molecular reaction dynamics directed by Professor Ian W M Smith and Dr Ian R Sims. The research, including the postdoctoral position, is funded by EPSRC and the project is entitled:

The Formation and Reactions of Hydrogen in Specific Rovibrational States

The fellow will develop state-of-the-art laser methods for preparing and detecting H₂ in specific rovibrational levels. These methods will then be used to determine state-to-state information about bimolecular reactions in which H₂ is a reagent or product, including the rate constants for reaction H₂ with atomic and diatomic free radicals and the product state distributions of H₂ formed in the reactions of H atoms with vibrationally excited H₂O and HCN.

The position is available from April 2000 for two years (one year renewable for a second). The exact starting date is negotiable. Applications are encouraged from candidates of any nationality.

Informal enquiries are welcome and should be directed to Professor Ian WM Smith FRS or to Dr Ian Sims.

This advert may also be found at <http://web.bham.ac.uk/i.r.sims/postdoc.htm>

Postdoctoral Position, International School for Advanced Studies in Trieste (Italy)

A postdoctoral position is available, starting immediately, for 1 year on a project entitled:

"Density-functional theory-based molecular dynamics simulations of biological systems"

The work will involve applications of the Car-Parrinello to systems of pharmaceutical relevance, such as targets for anti-AIDS and anti-cancer therapy.

For further information please send an email message to:

Dr. Paolo Carloni, International School for Advanced Studies, SISSA, via Beirut 4, 34014 Trieste, Italy

<http://www.sissa.it/cm/bc/>

email: carloni@sissa.it

Phone: +39-040-3787407, Fax:+39-040-3787528

Postdoc position; Hebrew University

A postdoc position is available starting Spring 2000 in the group of Prof. Uri Banin, at the department of Physical Chemistry in the Hebrew University of Jerusalem, Israel.

The research topic is the size dependent optical spectroscopy of semiconductor nanocrystals and semiconductor cluster-molecules, which manifest the transition from the molecular regime to the solid state. The project is a collaboration with the group of Prof. Dr. Dieter Fenske from the Institute of Inorganic Chemistry in Karlsruhe, Germany. Interest and experience in optical spectroscopy methods, including cryogenic methods, is desired.

The position is offered for two years, extended on a yearly basis. Interested candidates should send further inquiries, a CV, list of publications, and have two letters of reference forwarded to Uri Banin at the address given below.

Some recent publications related to the proposed project are: U. Banin et. al, Nature 400, 542-544 (1999).

M. Jacobsohn, U. Banin, J. Phys. Chem. B 104, 1-5 (2000).

Y.W. Cao, U. Banin, Angew. Chem. Int. Ed. Eng. 38, 3692-3694 (1999).

Dr. Uri Banin, Department of Physical Chemistry, The Hebrew University, Jerusalem 91904, Israel

TEL.:972-2-6584515, FAX: 972-2-5618033

Postdoctoral Position, National Tsing Hua University, Taiwan

A postdoctoral position in the area of gas-phase ultrafast reaction dynamics is available immediately at the Department of Chemistry, National Tsing Hua University, Taiwan. The postdoc will be expected to carry out experimental research based on femtosecond time-resolved photofragment translational spectroscopy, a relatively new and powerful technique in studying photodissociation dynamics. The experiments will use an amplified fsec Ti:sapphire laser system and a time-of-flight mass spectrometer operated under the energy-analyzing mode. The starting annual salary is about US24K. The initial appointment is for one year with the expectation of renewal for up to three years. Experience with ultrafast lasers and/or nsec laser-TOF-MS is desirable. Applicants should send a C.V. and arrange for at least two letters of recommendation to be sent to Prof. Po-Yuan Cheng, Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 30043 (e-mail:pycheng@mx.nthu.edu.tw, FAX:886-3-571-1082)

Postdoc positions: Theoretical/Computational Biophysics, SUNY Buffalo

Postdoctoral positions are available after July 1, 2000 at Center for Single Molecular Biophysics of Department of Physiology and Biophysics of SUNY Buffalo to conduct theoretical and computational research in biophysics. Qualified candidates should have a PhD in Chemistry, Physics. The university Center for Computational Research also has 128-processor Origin 2000, 28-processor SP2, and a cluster of 64 Sun Ultra 5 workstations. Please send your CV with cover letter, and the names, addresses, and phone numbers of two referees familiar with your work. Email to zhou@tammy.harvard.edu with plain text file or postscript file is preferred. Regular mail should send to Dr. Yaoqi Zhou, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford St. 232, Cambridge, MA 02138, or Department of Physiology and Biophysics, 124 Sherman Hall, University at Buffalo, State University of New York Buffalo, New York 14214 after July 1, 2000.

Postdoctoral Position, Brookhaven National Laboratory

A postdoctoral position is available in chemical dynamics involving thermal and photo-induced reactions of adsorbates on metal and metal-oxide surfaces. State-resolved probes of the desorbed products are used to study the charge and energy transfer processes induced by photoexcitation at the adsorbate-metal interface and the resulting reaction dynamics leading to desorption. This work is part of a larger interdisciplinary surface chemistry effort at Brookhaven which includes access to spectroscopy and structural beam lines at the National Synchrotron Light Source.

The successful candidate should have a background in laser-based chemical dynamics, surface (photo)chemistry or surface scattering. Experience with REMPI techniques, time-of-flight mass spectrometry or ion-imaging is also desirable. Brookhaven National Laboratory is an equal opportunity employer.

Applicants should send a CV and three letters of recommendation to: Michael G. White, Chemistry

Department, Brookhaven National Laboratory, Upton, NY 11973
Phone: (516) 344-4345; e-mail: mgwhite@bnl.gov

Postdoc Fellowship, Theoretical/Computational Chemistry, Taipei, Taiwan

A postdoc fellowship in theoretical/computational chemistry is available in the molecular modelling lab of the Sun group at the chemistry department of the National Taiwan Normal University. The Department of Chemistry is one of the most research-active institutes in Taiwan. Our laboratory equipped with excellent computing resource provides an excellent environment for theoretical study of the condensed phases systems and molecular systems. The current topics include 'vibrational dynamics on semiconductor surfaces', 'protein backbone dynamics and unfolding', and 'face selectivity of reactions using quantum chemistry calculation'. Applicants with expertise in theoretical/computational chemistry area are welcome to send your CV and three reference letters to Ying-chieh Sun at sun@scc.ntnu.edu.tw, or the address:

Department of Chemistry, National Taiwan Normal University, 88 Ting-Chow Road Sec. 4, Taipei, 11718, Taiwan, ROC

Fax: 886-2-2932-4249

For more info, please look up <http://140.122.142.51/~sungroup>

The salary for this position is about 22,000 US dollars per year. Chinese is the language everybody speaks. In the academic and research environment, there is no problem to communicate in English.

There are two channels for application of the postdoc positions. One is available immediately, the other is to apply these positions with applicant qualification and the projects he/she is going to work on. In the present case, I am going through the latter one this time at this moment of this fiscal year.

With the projects going on in my group and a suitable applicant's qualification, it is very much highly that the application will be approved if everything goes well. In this case, the postdoc fellowship will be available in about 3-4 months from the date of application.

Postdoctoral position, Universite de Liege, Belgium

A postdoctoral position is available for a period of twelve months starting around April 1, 2000 to investigate the dynamics of unimolecular reactions in ion beams. Particular attention will be paid to kinetic (translational) energy release distributions. The research will be conducted both at the experimental and theoretical level but the balance between experimentation and theory will be determined by mutual agreement. For some of our recent publications, see J. Chem. Phys. 110, 2911 (1999); Int. J. Mass Spectrom. 185/186/187, 155(1999); J. Chem. Phys. 111, 9259 (1999). Salary will be equivalent to that offered to the university staff at the same level of qualification. Applications coming from graduate students will also be considered. Send applications and CV indicating previous experience to Prof. J.C. Lorquet, Departement de Chimie, Universite de Liege, Sart-Tilman, Batiment B6, Liege 1, Belgium; Fax: 32-04-3663414 or 32-04-3662933; e-mail: jc.lorquet@ulg.ac.be. Arrange for recommendation letters to be directly sent either by regular mail, fax or e-mail to the same address.

Postdoctoral position at Leeds

A postdoctoral position is available in the femtosecond molecular dynamics group at Leeds University, UK. The project is focussed on the application of velocity map imaging (ion imaging) to Coulomb explosion pump-probe experiments on diatomic and triatomic molecules. A femtosecond laser is used to prepare an evolving wavepacket on a dissociative surface of the molecule. The time evolution is probed by the application of an intense ultra-short laser pulse (~5-10 mJ ~20 fs) after a controlled delay. The intense pulse induces a Coulomb explosion in the molecule by stripping the valence electrons from the molecule. The ions are imaged using velocity mapping and thus the nuclear configuration at the moment of ionisation can be deduced.

The femtosecond molecular dynamics group provides an excellent research environment with a well equipped laboratory. The three permanent members of the group are Prof. Godfrey Beddard, Dr. Benjamin Whitaker and Dr. Gavin Reid. Currently there are three other members in the team. The laboratory is equipped with two amplified femtosecond lasers (home built) and a velocity mapping molecular beam apparatus. A Terahertz imaging system is also likely to be sited in the laboratory in the near future.

Candidates should have strong experimental skills and the ability to work in a team environment. Experience of femtosecond laser systems would be an advantage but not essential given a strong background in chemical reaction dynamics or another area of chemical physics. The position is only open to non-UK European Union nationals (funding is through the EU TMR programme).

There are also openings for PhD students of any nationality.

Applications should be sent to:

Dr Benjamin J Whitaker, School of Chemistry University of Leeds, Leeds LS2 9JT, UK

tel: +44 113 233 6580, fax: +44 113 233 6565

web: www.chem.leeds.ac.uk

Further details about the TMR project can be found at <http://www.chem.leeds.ac.uk/IMAGINE>

b. Preprints

Coherence-controlled transparency and far-from-degenerate parametric gain in a strongly-absorbing Doppler-broadened medium

Optics Letters

Thomas F. George* and Alexander K. Popov

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

An inversionless gain of anti-Stokes radiation above the oscillation threshold in an optically-dense far-from-degenerate double-lambda Doppler-broadened medium accompanied by Stokes gain is predicted, where optical switching from absorption to gain via transparency controlled by a small variation of the medium and of the driving radiation parameters, which are at a level less than one photon per molecule, is shown for sodium dimer vapor.

New optical effect of diffractive multifocal focusing of radiation on a bicomponent diffraction system

Applied Optics

Renat R. Lettfullin and Thomas F. George*

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

It is shown that when a plane wave illuminates a certain type of bicomponent optical system, consisting of two plane screens with circular apertures on a given optical axis, a multifocal diffractive focusing effect can appear.

Dynamics of excitations in conjugated polymers and their response to an electric field

Trends in Chemical Physics

K. Chen, H. Jiang, X. Sun and Thomas F. George*

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

In a weak electric field, the exciton and biexciton have opposite responses to the electric field; but in a strong electric field, the exciton can be dissociated into two polarons with opposite charges.

Nonadiabatic transitions due to curve crossings: Complete solutions of the Landau-Zener-Stueckelberg problems and their applications.

Adv. Chem. Phys.

Chaoyuan Zhu, Yoshiaki Teranishi and Hiroki Nakamura*

Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan. nakamura@ims.ac.jp

Theoretical studies of multidimensional proton tunneling in the excited state of tropolone.

J. Chem. Phys.

Marek Wojcik, Hiroki Nakamura* and Suehiro Iwata

Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan. nakamura@ims.ac.jp

Nonadiabatic transitions in a Two-State Exponential Potential Model

J. Phys. A.

Lukas Pichl, Vladimir I. Osherov and Hiroki Nakamura*

Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan
A general two-state exponential potential model is investigated and the corresponding two channel problem is solved by means of semiclassical theory. The analytical expression for the nonadiabatic transition matrix yields a unified expression in the repulsive and attractive cases. The theory is demonstrated to work very well even at energies lower than the diabatic crossing region.

Quantum Reaction Dynamics of O(3P)+HCl on a New ab initio Potential Energy Surface

J. Chem. Phys.

Katsuyuki Nobusada, Hiroki Nakamura* Yogjing Lin and B.Ramachandran

Division of Chemistry, Graduate School of Science, Hokkaido Univ., Sapporo, Hokkaido 060-0810, Japan,
Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan,
Chemistry, College of Engineering and Science, Louisiana Tech Univ., Ruston, Louisiana 71272, USA

The quantum dynamics studies are made with use of the new surface calculated by Ramachandran et al. for $J=0$. The hyperspherical elliptic coordinates are used and reaction dynamics are clarified in terms of the previously established concept that reactive transitions are nothing but vibrationally nonadiabatic transitions at important avoided crossings in the vicinity of the potential ridge. Comparisons are with the previous calculations based on the KSG surface and the classical trajectory calculations.

Complete Reflection in Two-State Crossing and Non-crossing potential systems

J. Chem. Phys.

Lukas Pichl, Hiroki Nakamura* and Jiri Horacek

Department of Functional Molecular Science, The Graduate Univ. for Advanced Studies, Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan
Institute of Theoretical Physics, Charles Univ. Praha 8, 18000 Czech Republic

A semiclassical study is made for the complete reflection and transmission phenomena in two coupled potential systems. The conditions for these phenomena to occur are expressed analytically. Also introduced an exactly solvable model of diabatically avoided crossing. These models and phenomena may be useful in controlling various molecular processes in laser fields, since in the dressed or Floquet state formalism molecular potentials can be shifted up and down and are made to cross or avoid crossing with other potentials.

A QUASICLASSICAL TRAJECTORY STUDY OF THE H₂ + H₂ REACTION

Chem. Phys. Letters 305, (3-4) 276 - 284 (1999).

A. Ceballos, E. Garcia, A. Rodriguez, and A. Laganà,

Effect of translational energy and vibrational and rotational excitation on the efficiency of reactive, non reactive and dissociation processes.

INNOVATIVE COMPUTING AND DETAILED PROPERTIES OF ELEMENTARY REACTIONS USING TIME INDEPENDENT APPROACHES

Computer Physics Communications 116, 1-16 (1999).

Antonio Laganà

Parallel models for reactive scattering codes and the importance of decoupling in allowing efficient implementations on massively parallel architectures

THE INFLUENCE OF INITIAL ENERGY ON PRODUCT VIBRATIONAL DISTRIBUTIONS AND ISOTOPIC MASS EFFECTS IN ENDOERGIC REACTIONS: THE Mg + HF CASE

Phys. Chem. Chem. Phys. 1(6) 1133 - 1141 (1999).

F. Huarte-Larrañaga, X. Giménez, M. Albertí, A. Aguilar, A. Laganà and J.M. Alvarino

Mechanism favouring reaction and tunneling at threshold in heavy heavy light systems are intimately related to the orientation of the target molecule and to the mass of the colliding partners

ON THE OPTIMIZATION OF A PIPELINE MODEL TO INTEGRATE REDUCED DIMENSIONALITY SCHRÖDINGER EQUATION FOR DISTRIBUTED MEMORY ARCHITECTURES

The International Journal of Supercomputer Applications and High Performance Computing Applications 13(1), 49 (1999).

R. Baraglia, R. Ferrini, D. Laforenza, and A. Laganà,

The use of pipeline models in integrating two dimensional Schrödinger equations as an alternative to task farm models when memory requirements become too large is discussed. Sources of efficiency loss are examined in detail.

AN OPTIMIZED TASK-FARM MODEL TO INTEGRATE REDUCED DIMENSIONALITY SCHRÖDINGER EQUATIONS ON DISTRIBUTED MEMORY ARCHITECTURES.

Future Generation Computer Systems 15(4) 497-512 (1999).

R. Baraglia, R. Ferrini, D. Laforenza, A. Laganà,

The application of task farm parallel models to integrate reduced dimensionality scattering equations needs to be checked against the efficiency in assigning the computational load

QUANTUM REACTIVE SCATTERING CALCULATIONS

in High performance cluster computing - Vol. 2 B. Rajkumar Ed. chap. 28, 580-603 (1999), Prentice Hall PTR, 1999.

R. Baraglia, R. Ferrini, D. Laforenza and A. Laganà

Cluster computing as an alternative to parallel computing on homogeneous platforms is considered for reactive scattering calculations. The evaluation of the impact of computational bottle necks and proposal for their minimizations are considered

DOUBLE WELL STRUCTURE AND MICROSCOPIC BRANCHING IN THE $O(^1D)+HCl$ REACTION

Chem Phys Letters 313, 299 - 306 (1999).

José María Alvariño, Aurelio Rodríguez, Antonio Laganà and María Luz Hernández

The role played by the potential energy wells associated with stable reaction intermediates of the reaction mechanisms of the title reaction are considered not only with respect to the yield of different products but also in the different contributions to the internal energy distribution of the same product

ATTACK AND RECOIL ANGLE DEPENDENCE OF THE $Li + HF \rightarrow LiF + H$ REACTION AT $J=0$

J. Phys. Chem. 103, 10776-10782 (1999).

M. P. de Miranda, S. Crocchianti, A. Laganà,

Alternative approaches to the evaluation of stereodynamical effects for the title reaction are considered and related advantages and disadvantages are discussed.

COMPUTATIONAL GRANULARITY AND PARALLEL MODELS TO SCALE UP OF REACTIVE SCATTERING CALCULATIONS

Computer Physics Communications

A. Laganà, S. Crocchianti, A. Bolloni, V. Piermarini, R. Baraglia, R. Ferrini, D. Laforenza, Architectural features of parallel computers differently impact on the efficiency of a code when an application is scaled up. This reflects on the different suitability of computational approaches of well performing on these machines when the system to be treated becomes heavier or the quantity to be calculated changes.

QUASICLASSICAL TRAJECTORY SIMULATION OF THE $O(^1D) + HCl \rightarrow OH + Cl, ClO + H$ REACTIONS ON AN IMPROVED POTENTIAL ENERGY SURFACE

Phys. Chem. Chem. Phys. 2, 589 - 597 (2000).

T. Martinez, María Luz Hernández, José María Alvariño, Antonio Laganà, F.J. Aoiz, M. Menendez, and E. Verdasco

An extended study of the title reaction performed on an improved potential energy surface using quasiclassical means to compare theoretical predictions with quantities measured by the experiment

COMPUTATIONAL REACTION AND MOLECULAR DYNAMICS: FROM SIMPLE SYSTEMS AND RIGOROUS METHODS TO COMPLEX SYSTEMS AND APPROXIMATE METHODS

Lecture Notes in Chemistry xx, xx (2000)

A. Laganà, A. Riganeli

The increasing need for introducing approximations when moving from a few atom reactions to polyatomic systems is illustrated and the nature of the approximation discussed

ON THE EFFECT OF INCREASING THE TOTAL ANGULAR MOMENTUM ON Li + HF REACTIVITY

Chem. Phys. Letters (submitted)

A. Laganà, A. Bolloni, S. Crocchianti, G.A. Parker,

Quantum time independent calculations of the reactive probabilities of the Li + HF reaction have been performed for total angular momentum quantum numbers varying from 0 to 2. The relevance of including non zero total angular momentum contributions to the J shifting calculation of the cross section is analyzed with respect to its low energy structure.

QUASICLASSICAL AND QUANTUM RATE COEFFICIENTS FOR THE O + O₂ REACTION

Edito da A. Laganà (Università di Perugia, Perugia, 1999).

A. Laganà, E. Garcia and M.T. Martinez

Rate coefficients of the title reaction calculated as a function of reactant vibrational excitation and as a function of rotational and translational temperatures. The importance of potential energy wells to induce multiquantum vibrational deexcitation

Production, characterization and scattering of a sulfur atom beam: Interatomic potentials for the rare-gas sulfides, RS (R = Ne, Ar, Kr, Xe).

Phys. Chem. Chem. Phys.

Vincenzo Aquilanti^b, Daniela Ascenzi^b, Elisabetta Braca^c, David Cappelletti^{a,c}, and Fernando Pirani^{a,b}

^aINFN and ^bDipartimento di Chimica and ^cIstituto per le Tecnologie Chimiche, Università di Perugia, I-06100 Perugia, Italy

An intense and stable continuous beam of S atoms and SO radicals is produced from a microwave discharge source operating in a SO₂-He mixture. The S-atom beam, characterized by coupling mechanical velocity selection with magnetic analysis and detected by a quadrupole mass filter, has been employed in scattering experiments. Total integral cross sections for collisions of S (³P_j) atoms with Ne, Ar, Kr, and Xe have been measured in the beam velocity range 1.0 - 2.4 Km/s. The results are analysed to yield a characterization of the spherical and anisotropic components of the interaction, providing lengths and strengths of the bonds in the six low lying states of the rare-gas sulfides NeS, ArS, KrS and XeS.

Coupling by Charge Transfer: role in bond stabilization for open-shell systems and ionic molecules and in harpooning and proton attachment processes

Molecular Physics

F.Pirani, A.Giulivi, D.Cappelletti, V.Aquilanti

Dipartimento di Chimica, University of Perugia, Italy

A variety of phenomena of apparently different nature can be compacted and described within a unifying picture by taking into account the role of the charge transfer interaction. A proper representation is obtained both for the transition from van der Waals to chemical bonds and for the behaviour of different families of compounds, such as those of alkali halides and of rare-gas protonated systems. This paper is dedicated to the memory of Professor Roger Grice (1941–1998).

Sturmian expansion for quantum mechanical many-body problems, and hyperspherical harmonics

Adv. Quantum Chemistry

Vincenzo Aquilanti

Department of Chemistry, University of Perugia

John Avery

H.C. Ørsted Institute, University of Copenhagen

Generalized Sturmian basis sets make it possible to solve the many-particle Schrödinger equation directly, without the use of the self-consistent-field approximation.

The close relationship between generalized Sturmian basis functions and hyperspherical harmonics is discussed, as well as the relationship among all the matrix elements of the theory, such as the Shibuya-Wulfman integrals, the generalized Wigner coefficients of angular momentum theory, and the Hahn polynomials of modern numerical analysis.

Evidence for steric effect in methyl chloride ionization by metastable argon atoms

Chemical Physics Letters, 313 (1999) 484-490

H. Ohoyama, H. Kawaguchi, M. Yamato, T. Kasai

Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
B.G. Brunetti, F. Vecchiocattivi

Dipartimento di Chimica e Istituto per le Tecnologie Chimiche, Università di Perugia, 06123 Perugia, Italy

The orientation dependence of methyl chloride ionization by collision with metastable argon atoms at an average collision energy of 0.09 eV has been investigated using an electric hexapole field selector followed by an orienting field. The steric opacity function of the process has been determined. The highest reactivity has been found for approaches of the metastable atom towards the Cl-end of the molecule, while the lowest corresponds to the opposite approaches, close to the CH₃-end. The stereo-selectivity is discussed in terms of spatial distribution of the highest occupied molecular orbital of CH₃Cl, mainly localized on the chlorine atom.

Anisotropy effects in methyl chloride ionization by metastable neon atoms at thermal energies.

J. Physical Chemistry A. 104, 7, 1405-1415

M. Albertí, J.M. Lucas

Departament de Química Física i Centre Especial de Recerca en Química Teòrica, Universitat de Barcelona, Barcelona, Spain

B. Brunetti, F. Pirani, M. Stramaccia

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

M. Rosi, F. Vecchiocattivi

Istituto per le Tecnologie Chimiche, Università di Perugia, 06124 Perugia, Italy

Quasiclassical trajectories calculations have been carried out for the Penning ionization

$\text{Ne}^*(^3\text{P}_{2,0}) + \text{CH}_3\text{Cl} \rightarrow \text{CH}_3\text{Cl}^+(\text{X, A, B}) + \text{Ne} + \text{e}^-$. The calculations have been performed, within the rigid rotor approximation, for the translational energy range of 0.04-0.2 eV. The interaction potential of the colliding $\text{Ne}^*-\text{CH}_3\text{Cl}$

system has been semiempirically estimated. The ionization probability has been determined.

COLLECTIVE HYPERSPHERICAL COORDINATES FOR POLYATOMIC MOLECULES AND CLUSTERS

Mol. Phys.

Vincenzo Aquilanti, Andrea Beddoni, Simonetta Cavalli and Andrea Lombardi

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

Robert Littlejohn

Department of Physics, University of California, Berkeley, California 94720, USA

For n -body dynamics we analyze the properties of configuration space within a symmetric hyperspherical framework. Coordinates are conveniently broken up into spatial (or external) rotations, kinematic invariants (related to the inertia moments) and kinematic (or internal) rotations. Their usefulness is shown for the study of constrained intramolecular motions and of concerted reactions and for collective modes of polyatomic molecules and clusters. At a fixed hyperradius, which is a measure of total inertia, the space of kinematic invariants is the surface of a right spherical triangle that leads to the tetrahedral (for $n = 4$) or octahedral (for $n \geq 5$) tessellation of the sphere. Alternative parametrizations are discussed, including the proper one to deal with the umbrella inversion motion of ammonia.

Chemical reaction dynamics with molecular beams

Reports on Progress in Physics Vol. 63, pp. 355-414 (2000)

P. Casavecchia

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

This comprehensive review describes advances which have occurred during the past decade in chemical reaction dynamics using crossed molecular beams and laser techniques.

Cyanomethylene formation from the reaction of excited nitrogen atoms with acetylene: a crossed beam and ab initio study

J. Am. Chem. Soc. 122, 4443 (2000)

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

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

K. Sato

Department of Applied Physics, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo, 152-8551, Japan

T. Takayanagi and Y. Kurosaki

Advanced Science Research Center, Japan, Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan.

The results of a crossed beam study of the reaction of excited nitrogen atoms, $N(^2D)$, with acetylene, combined with electronic structure calculations and RRKM predictions allow us to identify cyanomethylene (HCCN) as the main primary reaction product and to establish its formation dynamics. The relevance of this reaction to the upper atmosphere of Titan is briefly discussed.

Observation of nitrogen bearing organic molecules from reactions of nitrogen atoms with hydrocarbons: A crossed beam study of $N(^2D) + \text{ethylene}$

J. Phys. Chem. A (Letters) 104, 5655 (2000)

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

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

The dynamics of the reaction of excited N atoms with ethylene is investigated by the crossed beam method. The N/H exchange channels, leading to 2H-azirine, ketenimine, and acetonitrile formation via a bound intermediate are found to be the main reaction channels. The relevance to Titans atmospheric chemistry is briefly discussed.

A crossed beam study of the reaction $C(^2D)+H_2 \rightarrow CH(v')+H$

Chem. Phys. Letters, submitted.

A. Bergeat, L. Cartechini, N. Balucani, G. Capozza, L. F. Phillips, P. Casavecchia*, and G.G. Volpi

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

L. Bonnet and J.-C. Rayez

Laboratoire de Physico-Chimie Moleculaire, Universit Bordeaux 1, 33405 Talence Cedex, France

Product angular and time-of-flight distributions have been measured for the first time for the prototypical insertion reaction $C(^2D)+H_2$ at the collision energy of 1.86 kcal/mol using the crossed beam technique. Center-of-mass angular and kinetic energy distributions have been derived for $CH(v'=0)+H$ products and compared with those of statistical calculations based on Phase Space Theory.

New way of controlling molecular processes by lasers "Quantum Control of Molecular Reaction Dynamics" edited by R.J.Gordon and Y.Fujimura (World Scientific,2000).

Yoshiaki Teranishi, Kuninobu Nagaya and Hiroki Nakamura*

Department of Theoretical Studies, Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan. nakamura@ims.ac.jp

c. Conferences

1. Atomic and Molecular Interaction (AMI) Gordon Conference.

This year's AMI Gordon Conference will be held at Colby Sawyer College in New London, New Hampshire from July 2nd to July 7th. The meeting will include 29 invited talks (Speaker list is below) on both

experimental and theoretical subjects associated with the conference title. Subjects to be covered at this year's meeting include; non-adiabatic processes, bimolecular and unimolecular reactions, surface/molecule interactions, chemistry in clusters, low-temperature chemistry and intra and inter molecular energy transfer. In addition there will be two poster sessions. All attendees, especially graduate students and postdocs, are encouraged to present a poster. Send poster abstracts to David W. Chandler at MS 9055, PO Box 969, Sandia National Laboratory, Livermore CA, 94551.

The Gordon Conference attendance will be limited to 120 participants including speakers. Those interested in attending please consult the Gordon Research Conference web pages:

<http://www.grc.uri.edu/> and <http://www.grc.uri.edu/programs/2000/atomic.htm>

To apply to attend the AMI-GRC, please fill out the email form at: app@grcmail.grc.uri.edu or by mail from: Conference Application Gordon Research Conferences University of Rhode Island P.O. Box 984 West Kingston, RI 02892-0984 USA 401-783-4011 401-783-7644 (FAX)

Invited Speakers List: Fred Temps (University Kiel, Germany) Ned Sibert (Univ. of Wisconsin, USA) Mike Ashfold (University of Bristol, England) Kopin Liu (IAMS, Taiwan) George Schatz (Northwestern University, USA) David Parker (Univ. of Nijmegen, the Netherlands) Steve Gray (Argonne National Laboratory, USA) David Nesbitt (Univ. of Colorado, USA) Michael Collins (Australian National University, Australia) Piero Cassavechia (Univ. of Perugia, Italy) Carl Hayden (Sandia National Laboratory, USA) Kirk Peterson (Pacific Northwest Laboratory, USA) Wei Kong (Oregon State University, USA) Antonio Lagana (University of Perugia, Italy) Jim Valentini (Columbia University, USA) Octavio Roncero (I.M.A.F.F. (C.S.I.C.), Spain) Curt Wittig (University of Southern California, USA) Greg Sitz (University of Texas, USA) Bret Jackson (University of Massachusetts-Amherst, USA) Arthur Utz (Tufts University, USA) Anthony Stone (Cambridge, England) Mike Pilling (Univ. of Leeds, England) Eric Herbst (Ohio State University, USA) Ian Smith (Univ. Birmingham, England) Charlie Parmenter (Indiana University, USA) Ad van der Avoird (Univ. of Nijmegen, the Netherlands) Steven Stolte (Free University of Amsterdam, The Netherlands) Jeremy Hutson (University of Durham, England) George Ewing (Indiana University, USA) Conference Chair: David W. Chandler, Sandia National Laboratory, PO Box 969, MS 9055, Livermore CA, 94551-0969, chandler@ca.sandia.gov, FAX:925-294-2276

Vice Chair: Albert F. Wagner, Argonne National Laboratory, Argonne IL, 60439, wagner@anchim.chm.anl.gov

2. Summer School on "Atomic Clusters and Nanoparticles"

ECOLE D'ETE DE PHYSIQUE THEORIQUE, LES HOUCHES, in the French Alps, July 3-28, 2000. The Director is Claude Guet, CEA, Grenoble. The Organizing Committee consists of R. S. Berry, F. David, C. Guet, P. Hobza, J. Jortner and F. Spiegelmann.

The school aims at providing advanced doctoral and postdoctoral researchers with the state of the art of theoretical concepts and methods that have become extremely powerful in investigating the structure, dynamics, kinetics and thermodynamics of atomic and molecular clusters and nanoparticles.

Participation will be international. There will be a limit of 50 students, due to the amount of space available at the Ecole. The school will be 4 weeks long.

FOR DETAILS AND APPLICATION FORMS, GO TO THE WEB SITE!

<http://w3houches.ujf-grenoble.fr/session-73/shtml>

3. Annual Northern Universities (Informal) Meeting on Chemical Physics

(supported by the Chemical Physics Group of the IOP) to be held on Tuesday July 11th, 2000 10.00am - 5.00 pm at the University of Liverpool

As at previous meetings this will be an informal meeting of researchers from the Midlands, Scotland and the North of England, where young researchers can talk about their work in a friendly environment. This event covers all aspects of chemical physics.

Offers of talks and/or posters are now invited. Please respond by Friday June 23rd at the latest.

Talks - should be 15-20 mins.

Posters - there will be space for posters and the session will take place over lunch.

Registration costs - including coffee, tea and a sandwich lunch - 5 stlg to be paid on the day.

Please respond by filling in the registration form below and returning to either

andrewh@ssci.liv.ac.uk or june.mccombie@nottingham.ac.uk

Registration Form

Annual Northern Universities (Informal) Meeting on Chemical Physics

Tuesday July 11th, 2000 10.00am - 5.00 pm, University of Liverpool

I will / will not be attending the meeting

I will be bringing with me colleagues.of these are vegetarian / vegan (or have other dietary requirements (please specify).

Talks are offered by:

Name:

Title:

Posters are offered by:

Name:

Title:

4. 16TH INTERNATIONAL SYMPOSIUM ON GAS KINETICS

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

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

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

The scientific programme will include sessions on:

Dynamics and Kinetics of Elementary Reactions

Atmospheric Chemistry

Combustion and Dynamics

Inter- and Intra- Molecular Energy Transfer

Chemistry in Extreme Environments

Plenary Lectures will be given by D.J. Nesbitt, M. Brouard, J.N. Crowley, C.E. Kolb, C.T. Bowman, P.J.

Dagdigian, R.E. Miller and P. Andresen. The Polanyi Lecture will be presented by J. Wolfrum and is entitled:

"Laser Studies of the Kinetics of Homogeneous and Heterogeneous Processes: From Diatomics to DNA"

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

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

Completed forms may be submitted by email to: gk2k@atm.ch.cam.ac.uk

Alternatively forms may be posted to:

Gillian Southwell, 16th International Symposium on Gas Kinetics, University Chemical Laboratory,

Lensfield Road, Cambridge, CB2 1EW, U.K. (FAX +44 1223 336362). Registrations should be returned by:

FRIDAY JANUARY 7TH 2000

A full social programme is also planned, including tours of the Cambridge Colleges, a recital in King's College Chapel and a banquet in Robinson College Cambridge, where participants will be accommodated.

Dr David Husain has kindly agreed to give the post-banquet speech.

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

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

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

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

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

5. FEMTOCHEMISTRY AND FEMTOBIOLOGY EL ESCORIAL SUMMER SCHOOL 2000

Summer School July 24-28, 2000, El Escorial, Madrid (Spain)

Organized under the auspices of: Fundacion General de la Universidad Complutense de Madrid.

Co-sponsored by the European Science Foundation- ULTRA Network (Femtochemistry and Femtobiology) and by Bio-Rad Espana, Bruker Espanola, Innova and Lasing.

Chairmen: Jesus Santamaria and Luis Banares; Departamento de Quimica Fisica I; Facultad de Ciencias Quimicas; Universidad Complutense; 28040 Madrid, Spain

Secretary: Ignacio Sola; Departamento de Quimica Fisica I; Facultad de Ciencias Quimicas; Universidad Complutense; 28040 Madrid, Spain

Lecturers: Bruce Craig (Spectra-Physics, Mountain View, USA); Abderrazzak Douhal (Univ. Castilla-La Mancha, Toledo); Volker Engel (Wuerzburg, Germany); Jose M. Fernandez Corrales (Bio-Rad Espana, Madrid); Gustav Gerber (Wuerzburg, Germany); Joern Manz (Berlin, Germany); Octavio Roncero (CSIC, Madrid); Javier Solis (CSIC, Madrid); Ignacio Sola (Complutense, Madrid); Villy Sundstroem (Lund, Sweden).

Scientific programme: The school will be dedicated to provide an overview of the most recent advances in the fields of Femtochemistry, Femtobiology and Femtophysics. The course will cover experimental and theoretical aspects on femtosecond laser technology, gas phase reaction dynamics, reaction dynamics in condensed phases, proton and electron transfer, photoisomerization, primary steps in photosynthesis and vision, femtosecond multiphoton confocal microscopy, control of molecular processes, wavepacket dynamics, semiconductor clusters and nanocrystals, solid phase dynamics and ultrafast phase transitions.

Registration: The school is opened to about 60 graduate students and post-doctoral young researchers, both theoretical and experimental, in the fields of Femtochemistry, Femtobiology and Femtophysics. The registration fee is 21,000 Spanish Pesetas. Lodging and full board is available at the price of 46,000 Spanish Pesetas.

Grants from the Complutense University and from the European Science Foundation through the ULTRA programme (member organizations are Austria, Belgium, the Czech Republic, Denmark, Finland, France, Germany, Hungary, Italy, The Netherlands, Norway, Portugal, Sweden, Switzerland, Turkey and the United Kingdom) are available for graduate and post-doctoral students upon request. Deadline for grant applications: June 5, 2000; candidates should send a short Curriculum Vitae (via email; Latex, word, ...) to: Luis Banares (banares@legendre.quim.ucm.es) or Ignacio Sola (ignacio@tchiko.quim.ucm.es).

More information (in Spanish): <http://www.ucm.es/cursosverano>

6. MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS GORDON RESEARCH CONFERENCE

Colby Sawyer College, New London, New Hampshire July 30 - August 4, 2000 The scientific program will include 22 invited 40 minute talks arranged into the following sessions: Herzberg Session, From Atom-in-Molecule to Supercritical Fluids, Imaging and Control, Quantum Dots, A Little of This and A Little of That, Light Harvesting Antenna Systems, and Time vs. Frequency Domains. In addition there will be four poster sessions. All attendees, especially graduate students and postdocs, are encouraged to present a poster. Grant applications are pending which would provide partial support (Conference Fee and travel) for early-career scientists who plan to present a poster. The Invited Speakers include: Ch. Jungen, F. Merkt, R. Lipson, W. Ketterle, A. Vilesov, T. Momose, J. Brennecke, C. Hayden, C. Blondel, P. Bucksbaum, S. Leone, J. Cao, U. Banin, M. Moskovits, P. McEuen, H.F. Davis, M. Gruebele, R. Van Grondelle, K. Schulten, S. Volker and D. Jonas.

To apply to attend, the MES&D - GRC, please fill out the form obtainable by email at:

app@grcmail.grc.uri.edu

or request a form from Conference Application

Gordon Research Conferences

University of Rhode Island

P.O. Box 984 West Kingston, RI 02892-0984 USA

401-783-4011, 401-783-7644 (FAX)

<http://www.grc.uri.edu/programs/2000/molspec.htm>

Conference Chair: Robert W. Field, Room 6-219, MIT, 77 Mass. Ave., Cambridge, MA 02139 (617) 253-1489 (VOX), (617)-253-7030 (FAX), rwfield@mit.edu

Vice Chairs: Elliot Bernstein, Department of Chemistry, Colorado State University, Fort Collins, CO 80523-1872 (970) 491-6347 (VOX) (970) 491-1801 (FAX) erb@lamar.colostate.edu

James Skinner, Department of Chemistry, University of Wisconsin, Madison, WI 53706-1396 (608) 262-0481 (VOX) (608) 262-9918 (FAX) skinner@chem.wisc.edu

7. ATOMIC AND MOLECULAR DATA FOR ASTROPHYSICS NEW DEVELOPMENTS, CASE STUDIES AND FUTURE NEEDS. JOINT DISCUSSION

JD 1, August, 9-11, 2000 at the XXIVth GENERAL ASSEMBLY of the INTERNATIONAL ASTRONOMICAL UNION MANCHESTER, AUG. 7-18, 2000

Organized by IAU Commission 14: Atomic and Molecular Data Co-supporting Commissions: 15 (Physical Study of Comets, Minor Planets and Meteorites), 16 (Physical Study of Planets and Satellites), 29 (Stellar Spectra), 34 (Interstellar Matter), 36 (Theory of Stellar Atmospheres), 40 (Radio Astronomy), 44 (Space and High Energy Astrophysics).

MOTIVATIONS

The past few years have seen tremendous advances in observational techniques, both in space and on the ground. In the near future, several new ambitious and expensive spaceborne and ground based instruments will become available and provide a wealth of high quality observations in an extended range of wavelengths. The reduction, analysis and interpretation of the observational results requires, at each stage, increasingly extensive sets of atomic and molecular data especially since the objects studied are often in extreme physical conditions which cannot be reproduced in the laboratory and can be studied only by modelling. In this respect, it is the function of Commission 14 of the IAU to help keep the astronomers informed of the available data and of the programs undertaken in other communities, to favour the exchange of information in order to make the Atomic and Molecular Physics community aware of the needs of Astronomy for new data and, finally, to inform the program agencies of the needs for specific studies and funding in these areas. To this end, Commission 14 organizes a Joint Discussion at the next General Assembly of the IAU. The program is organized around topics corresponding to future or recent space missions or selected because they are fast moving and particularly in need of new laboratory data. In addition, case studies are included in which a particular species or process is analyzed from several angles in order to highlight its contribution to the interpretation of different astronomical observations or models. It is comprised of invited oral presentations and contributed posters.

Oral presentations and poster abstracts will be published in the proceedings to appear in:

Highlights of Astronomy (Vol. 12), 2000, J. Andersen Ed., PASP (San Francisco)

SCIENTIFIC ORGANIZING COMMITTEE:

S.K. ATREYA (USA), K.A. BERRINGTON (UK), J. CERNICHAO (Spain),
TH. HENNING (Germany), S. JOHANSSON (Sweden), T. MILLAR (UK),
F. ROSTAS (France, Chairperson), S. SAITO (Japan), D. SCHULTZ (USA),
P.SMITH (USA, Co-Chairperson), W.- L. TCHANG-BRILLET (France, Editor),
E. VAN DISHOECK (Netherlands)

CONTACT ADDRESS:

Francois ROSTAS, Observatoire de Paris-Meudon, 92195 Meudon Cx, France.

Telephone: +33 (0)1 45 07 75 65, Facsimile: +33 (0)1 45 07 71 00

e-mail: Francois.Rostas@obspm.fr

WEBSITE: <http://www.obspm.fr/IAU14/jd1.html>

VENUE, REGISTRATION, ABSTRACT SUBMISSION, TRAVEL GRANTS:

Please visit our website for details.

DEADLINES:

Peregistration: As soon as possible.

Application for travel grants: February 15, 2000.

Poster abstracts: February 15, in preliminary form, especially for grant applicants May 15 in final form for all participants.

Registration to the IAU General Assembly: Reduced rate: May 1, 2000.

SCIENTIFIC PROGRAM (as of January 28, 2000)

WEDNESDAY, AUGUST 9, MORNING

GRAINS

Grains in Astronomy:

Overview A. Witt (USA)

The Formation and Evolution of Interstellar Dust A. Jones (France)

Laboratory Analogues of Cosmic Dust H. Mutschke (Germany)

"GEMS" J. Bradley (USA)

INFRARED OBSERVATORIES (ISO / SOFIA / SIRTIF / FIRST)

Introduction E. vanDishoeck (Netherlands)

Infrared Observations of Ices A. Boogert (USA)

PAHs T.B.A

Silicates R. Waters (Netherlands)

Gas-phase Atomic and Molecular Species J. Lacy (USA)

THURSDAY, AUGUST 10, AFTERNOON POSTER SESSION

FRIDAY, AUGUST 11, MORNING GAS-SURFACE REACTIONS

Surface Reactions in Interstellar Space E. Herbst (USA)

Theoretical Simulations J. Takahashi (Japan)

Grain Surface Chemistry and Solid State Photochemistry W. Schutte (Netherlands)

H₂ IN SPACE D.R. Flower(UK)

THE WATER MOLECULE

H₂O in Young Stellar Objects T.B.A.

H₂O in the Sun and Stars P. Bernath (Canada)

H₂O in Comets, Observations and Models J. Crovisier (France)

ASTRONOMY, PHYSICS AND CHEMISTRY OF H₃⁺ T. Oka (USA)

FRIDAY, AUGUST 11, AFTERNOON

THE FUSE SPACE MISSION,

Atomic and Molecular Data, Needs and Availability K. Sembach (USA)

THE CHANDRA, ASTRO-E AND XMM SPACE MISSIONS,

Atomic Data for X-ray Astronomy N. Brickhouse (USA)

THE FERRUM PROJECT

New Experimental f-values for FeII S.Johansson (Sweden)

SOLAR SYSTEM MISSIONS

Laboratory Data for Exobiologically Oriented

Studies of Titan F. Raulin (France)

Laboratory Chemical Kinetics and Outer Planets R. Kaiser (China, R)

IR spectroscopy and Jupiter P. Drossart (France)

Clouds and Chemistry of Jupiter's Atmosphere S. Atreya (USA)

Atmospheric Probes T. Owen (USA)

POSTER CONTRIBUTIONS

Poster contributions by all participants are heartily encouraged as useful complements to the oral presentations. In particular, information and demonstrations concerning data bases are welcome.

It is planned to publish the poster abstracts in the proceedings of the Joint Discussion which will appear in Highlights of Astronomy (Vol. 12).

Preliminary abstracts should be submitted before February 15, 2000.

Final abstracts in LaTeX form must be received before May 15, 2000

For details, please visit our website: <http://www.obspm.fr/IAU14/jd1.html>

8. Symposium at the ACS National Meeting

This year at the ACS National Meeting in Washington, D.C. August 20-24, there will be a symposium to honor Ahmed H. Zewail, the 1999 Chemistry Nobel Laureate.

Professor Zewail received the Nobel Prize for "his studies of the transition states of chemical reactions using femtosecond spectroscopy," and the development of Femtochemistry.

Some of the invited speakers for this symposium are T. Baumert, A. W. Castleman, M. El-Sayed, M. Gruebele, V. B. McKoy, H. A. Rabitz, and N. F. Scherer.

In addition to the invited talks, there will be time for oral as well as poster contributions related to this symposium. I encourage you to submit an abstract.

Please submit your abstracts for oral or poster contributions electronically by April 15, 2000. Information about the ACS meeting can be found at <http://www.acs.org/meetings/washington2000/>

If you are interested in participating in this symposium or if you have experienced difficulties with the electronic submission process read on.

This year at the ACS National Meeting in Washington, D.C. August 20-24, there will be a symposium to honor Ahmed H. Zewail, the 1999 Chemistry Nobel Laureate. In addition to the invited talks, there will be time for oral as well as poster contributions related to this symposium. I encourage you to submit an abstract.

The deadline for oral or poster contributions is April 15, 2000.

To submit:

1. go to: <http://acs.confex.com/oasys.htm>

2. select Division of Physical Chemistry

3. Chose the symposium. You can submit for oral or poster presentation.

* Oral: Femtochemistry: 1999 Nobel Prize Symposium Ignore the 'only invited papers only' sign. There will be some time available for contributed talks.

* Poster Session: Femtochemistry

4. Continue according to their directions.

I hope this works for you and/or your students.

Additional information about the ACS meeting can be found at <http://www.acs.org/meetings/washington2000/>

Try to avoid the 'last day' rush.

Please let me know if you have a problem submitting an abstract.

Best Wishes,

Marcos Dantus Associate Professor

9. THE BRIJUNI CONFERENCE BRIJUNI (BRIONI) ISLAND, CROATIA

28.August-1.September 2000 Important problems for the XXI century

Important problems that confront science in future will be reviewed at the THE BRIJUNI CONFERENCE.

The scope is limited to some areas of science, and omission of very important other issues does not mean ignorance but rather limited time available. The issues that will be reviewed are: its structure and how to explore it. Fundamental properties of matter and materials is there room for radically new ideas where do we come from and where do we go to? At the conference the discussion periods are assigned significant lengths of time and the oral presentations are designed to form a framework for meaningful discussion. Apart from the usual aim of developing an up-to-date perspective of the present state of a given topic, the fundamental scientific philosophy behind the series of conferences is the stimulation of cross-disciplinary flow of knowledge and expertise from both the experimental and theoretical standpoints.

General information: Apart from the invited presentations there will be both oral and poster contributions; however the number of oral presentations will necessarily be limited. The registration fee is \$180 (\$60 students). For more details and the updated information see:

<http://www.brijuni-conference.irb.hr>

Deadlines: The conference attendance is limited to 80 participants (excluding accompanying guests). As a consequence it is important that, if you wish to participate, you should return the form below as soon as possible, preferably by 1 May 2000 and certainly no later than 1 Jun 2000 when the final reservations at the

Brioni Conference Centre must be confirmed. Please indicate below how certain you are of coming in the event that the conference is oversubscribed.

Application should be sent by email to: dbosanac@faust.irb.hr
or alternatively to the address:

S. Danko Bosanac
Institut Rugjer Boskovic
10001 Zagreb
Croatia
Tel: +385 1 4561 038
Fax: +385 1 4680 245

10. The 16th International Conference on High Resolution Molecular Spectroscopy Prague, Czech Republic, September 3-7, 2000

LOCAL ORGANIZING COMMITTEE

VLADIMIR SPIRKO, chairman, STnPAN URBAN, executive chairman, Academy of Sciences of the Czech Republic, J. Heyrovsky Institute of Physical Chemistry, Dolejskova 3, CZ-18223 Praha 8, Czech Republic
Tel.: +420 2 6605 3635, Fax: +420 2 858 2307 E-mail: paha2k@jh-inst.cas.cz

OTA BLUDSKY, SVATOPLUK CIVIS, PAVEL KUBAT, JITKA ONDRACKOVA, IVANA PAIDAROVA, PETR PRACNA, MARIE SIMECKOVA, MILAN SINDELKA, KAREL VOLKA, IVAN WILHELM, ZDENEK ZELINGER.

INTERNATIONAL STEERING COMMITTEE

PER JENSEN, chairman

FB 9 - Theoretische Chemie

Bergische Universitaet - Gesamthochschule Wuppertal

Gaussstrasse 20, D-42097 Wuppertal, Germany

Tel.: +49 202 439 2468, Fax: +49 202 439 2581, E-mail: paha2k@uni-wuppertal.de

JOSEF PLIVA (honorary chairman), LUCIANO FUSINA, VALERY I. PEREVALOV, GERARD PIERRE, WOLFGANG STAHL, JAMES K. G. WATSON.

2ND CIRCULAR: MARCH 2000

The conference will be held in Prague-Troja [approx. 5 km north of Wenceslas Square and less than 1 km from the Metro (subway/underground) station Nadrazi Holesovice], in buildings of the Charles University. The local organization will be undertaken by the J. Heyrovsky Institute of Physical Chemistry in the Academy of Sciences of the Czech Republic, Prague.

Please note that the meeting starts on a Sunday and ends on a Thursday. Hence you can conveniently make use of low-priced air line tickets requiring you to spend a Saturday night in Prague.

Please note that EUCMOSXXV: 25th European Congress on Molecular Spectroscopy will take place in Coimbra, Portugal, August 27 - September 1, 2000, that is during the week before PRAHA2000.

Prague, the capital of the Czech Republic, is a first-rank European cultural centre. It is not only a historical city with an extensive legacy of gothic and baroque cultural treasures, but also a modern metropolis with an infrastructure prepared to welcome more than a million visitors per year.

Scientific program

The invited speakers are:

DIONISIO BERMEJO, Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Double resonance Raman-Raman spectroscopy.

CLAUDE CAMY-PEYRET, Universite Pierre et Marie Curie, Paris, France: An overview of infrared spectrometry measurements for atmospheric science.

PAUL J. CRUTZEN, Otto-Hahn-Institut, Mainz, Germany: No title available.

THOMAS GIESEN, Universitaet zu Koeln, Germany: High resolution spectroscopy of pure carbon chain molecules.

MICHEL HERMAN, Universite Libre de Bruxelles, Belgium: No title available.

UFFE GRAAE JORGENSEN, Niels Bohr Institute, Copenhagen, Denmark: Spectroscopy of cool stars.

KEVIN K. LEHMANN, Princeton University, New Jersey, U.S.A.: Spectroscopy and dynamics of doped He nanodroplets.

ANTHONY J. MERER, University of British Columbia, Vancouver, Canada: Vibronic coupling effects in the electronic spectra of some polyatomic metal-containing radicals

THOMAS R. RIZZO, Ecole Polytechnique Federale de Lausanne, Switzerland: Multiple-resonance spectroscopy at chemically significant energies.

WILLIAM C. STWALLEY, University of Connecticut, U.S.A.: Photoassociative spectroscopy of ultracold atoms and formation of ultracold molecules.

KEIICHI TANAKA, Kyushu University, Fukuoka, and Institute for Molecular Science, Okazaki, Japan: Submillimeter-wave Spectroscopy of Floppy Molecules, - Proton Tunneling and van der Waals Vibration.

VLADIMIR G. TYUTEREV, Universite de Reims, France: No title available.

The lecture titles are preliminary.

Contributions, which will be presented partly as posters and partly as contributed lectures, are invited in the fields of:

* Observation, measurement, and analysis of high resolution rotational, vibrational, or electronic spectra of molecules (radicals, ions, complexes, clusters, ...) in the gas phase or in matrices.

* Experimental techniques for observing such spectra.

* Theory assisting the prediction, simulation, and interpretation of them.

* Applications in related fields such as the physics and chemistry of the atmospheres of planets and cool stars, the physics and chemistry of the interstellar medium, chemical kinetics, etc.

Abstracts

The deadline for submission of abstracts is May 1st 2000.

For more information access the PRAHA2000 WWW site at <http://www.chem.uni-wuppertal.de/conference/>

11. Faraday Discussion 117 - EXCITED STATES AT SURFACES

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

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

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

Experimental and theoretical contributions relating to the above areas or to any other, unmentioned, aspects of excited states at surfaces will be most welcome.

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

ORGANISING COMMITTEE

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

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

12. A Joint Meeting of CCP7 and the Astrophysical Chemistry Group

Observation, Analysis and Theory of Astronomical and Laboratory Spectra

6th - 8th September 2000, University of Kent at Canterbury

A joint meeting between CCP7 and the Astrophysical Chemistry group of the Royal Society of Chemistry will be held at the University of Kent at Canterbury on 6th - 8th September 2000. We have invited a galaxy of international speakers to the meeting to give lectures on all aspects of the Conference, including two tutorial lectures. The speakers and provisional lecture titles are:

Professor Pat Thaddeus: Carbon Chain Molecules

Professor Ted Snow: Results from FUSE

Professor Françoise Combes: Extragalactic Molecules

Professor Therese Encrenaz: Molecules in the Giant Planets

Dr Pascale Ehrenfreund: Ices observed by ISO

Professor Thomas Henning: Interstellar Dust

Professor Jonathan Tennyson: Calculating spectra for laboratory and astrophysical molecules

Dr Juliet Pickering: Laboratory spectroscopy

Dr Stephen Price: Formation of molecules on surfaces

Dr Jeremy Yates: Tutorial Lecture

Dr Tony Lynas-Gray: Tutorial Lecture

If you are interested in attending the Conference and presenting a paper or poster please check the Conference web site for an application form. Full details for the Conference can be found on the web site at <http://www.soton.ac.uk/~ams1/k2k>

If you have any further questions please send me an e-mail. (My apologies if you have received more than one copy of this announcement.)

Dr Andrew Shaw, Secretary to the Organising Committee

Dr Andrew M. Shaw Stanford University Department of Chemistry Stanford CA 94305-5080 Tel: 650-723-4335 Fax: 650-725-0259

13. Symposium for Theoretical Chemistry

Registration is now open for the 36th Symposium for Theoretical Chemistry, "Quantum Mechanics and Quantum Effects in Systems of Increasing Complexity" to be held in Litschau, Austria, from 10 to 14 September 2000.

REMINDER - PLEASE NOTE THE FOLLOWING DEADLINES

Registration (definitive booking): 20 June 2000

Poster/contributed talk (preliminary title): 20 May 2000 (due now!!!)

Poster/contributed talk (final title and abstract): 07 July 2000

THIS IS A FINAL CALL FOR CONTRIBUTED PAPERS

In case you wish to present a poster/contributed talk at STC2000, please

* either register now

* or register later but submit a preliminary title, as soon as possible, to stc2000.theor-chemie@univie.ac.at

Full information on STC2000 can be found on the home page: <http://www.itc.univie.ac.at/~STC2000/>

With apologies for possible cross-posting, and with further apologies and thanks to all those who have already sent in their contributions

14. European Summerschool in Quantum Chemistry (ESQC-00)

Riolo Terme, Italy September 17-30, 2000

The European summerschool in quantum chemistry (ESQC-00) will be arranged for the seventh time in September 2000. This 'extra' summer school will be arranged in Italy as a collaboration between the

Universities of Bologna and Lund (ESQC is normally arranged every odd year in Sweden. The next 'ordinary' school will be arranged in 2001). The school is open to students from all over the world, but some priority will be given to participants from the southern and eastern parts of Europe. A number of scholarships will be available to support students who have difficulties in financing their participation. The total number of participants is limited to 70 and the organizers will make the final selection of students in case there are more applicants. ESQC-00 will be arranged at the same level as earlier summer schools and with the same schedule. The only difference is the location.

The school will be arranged in the village Riolo Terme, located in Romagna on the eastern slopes of the Appenines between Bologna and Rimini.

The deadline for the preliminary registration is Jan 31, 2000.

Organizing Committee

Professor Gian Luigi Bendazzoli (University of Bologna)

Doctor Laura Gagliardi (Local Organizer, University of Bologna)

Professor Paolo Palmieri (University of Bologna)

President Gino Pasotti (IPS-International Products & Services, Milano and Terme di Riolo Bagni S.p.a., Riolo Terme, Italy)

Professor Bjrn O. Roos (School Director, Lund University)

The URL of the ESQC-00 Homepage:

<http://www.teokem.lu.se/esqc/00>

15. MOLEC 2000 (THE XIIIth MOLEC)

Jerusalem, Israel, September 17 - 22, 2000

Steering Committee: V. Aquilanti, M. Ashfold, M. Baer, K. Bergmann, G.D. Billing, G. Delgado-Barrio, F. Gianturco, Z. Herman, R. McCarroll, V. Sidis, J.P. Simons, S. Stolte, J.P. Toennies.

Local Organizing Committee: Michael Baer (Chair), Y. Band, R. Kosloff, A. Lifshitz, N. Moiseyev, A. Nitzan, E. Pollak, S. Rosenwaks, A. Wilson-Gordon, D. Zajfman.

General Information: MOLEC 2000 will be held in Jerusalem starting September 17 and ending September 22, 2000. The venue is the 4-star hotel of Kibbutz Ramat Rachel, on the Jerusalem municipal border. The Meeting, the XIIIth in the series of MOLEC conferences, will follow in format the former conferences.

Registration will be on Sunday, September 17 starting in the afternoon. There will be two morning sessions and two afternoon sessions on the Monday, Tuesday and Thursday. Wednesday afternoon will be free, for the excursion-tour (in Jerusalem). The Farewell dinner will be held Thursday night. Friday will be a half-day and the Meeting will end after lunch. All sessions will be plenary sessions. There will be three Poster sessions.

Invited speakers (confirmed so far): L.H. Andersen, V. Aquilanti, M. Barat, S. Berry, G.D. Billing, M.S. Child, L.S. Cederbaum, P. Crutzen, A. Dalgarno, G. Delgado-Barrio, A. Gonzales-Urena, G. Hancock, S. Haroche, Z. Hennis, J. Jortner, Y.T. Lee, C. Leforestier, R.D. Levine, C. Lifshitz, N. Makri, H.-D. Meyer, W.H. Miller, H. Nakamura, C.Y. Ng, B.J. Orr, M. Parrinello, U. Peskin, A.J.C. Varandas, and D. Yarkony. Progressive Registration Fee Deadlines: Normal rate: Up to 31/03/00: US \$200; up to 31/05/00: US \$250; after 01/06/00: US \$300. Student rate: Up to 31/03/00: US \$125; up to 31/05/00: US \$150; after 01/06/00: US \$175. Accompanying person: US \$50

Call for papers The topics covered by the conference include Reactive molecular collisions, Atmospheric chemistry, Astro-chemistry, Laser chemistry, Collisional energy exchange, Ion-molecule interactions, Electronic nonadiabatic effects and transitions, Collisions with surfaces and adsorbed species, Cluster studies, Photodissociation dynamics, Photodissociation and desorption at surfaces, Control of chemical processes, Doubly charged negative ions, Reactions in solution, Plasma, Ultra-cold atomic and molecular collisions, Resonance phenomena in molecular systems, Dissociative collisions, Unimolecular reactions, Molecular dynamics in dissipative systems. The submission of abstracts is encouraged. Some contributions may be selected for oral presentation. Deadline for abstracts: July 15, 2000.

A Last Announcement has been circulated, with registration form and hotel reservation form. Should you wish to receive the Announcement or if you want to inquire about the meeting please contact Michael Baer (mmbaer@netvision.net.il).

You are invited to visit the Conference website: <http://www.fh.huji.ac.il/~roib/MOLEC/index.htm> The Registration Form and the Form for Hotel Accommodations bookings may be downloaded from that site.

16. Chemistry and the Internet - ChemInt2000

This note is to announce that web Abstract Submission form is now operational for the Chemistry and the Internet (ChemInt2000) meeting being held in at Georgetown University in Washington DC on September 23-26, 2000.

The draft program of invited speakers, workshops, markup language tutorial, and panel sessions is available on the meeting web site: <http://www.chemint.org>

You are urged to look at the program and to consider submitting a poster paper to the meeting. Some 8-10 of poster papers will be selected for oral presentation at the meeting.

The main lecturers for the meeting will be:

Rene DePlanque, FIZ - Berlin

Jim Myers, Pacific Northwest Labs

Glen Hopkinson, Synopsys Scientific Systems

Wolf-Dietrich Ihlenfeldt, University of Erlangen-Nuremberg

Jim Ostell, NIH/NLM/NCBI

Engelbert Zass, ETH

Henry Rzepa, Imperial College, London

Peter Murray-Rust, Nottingham University

The (current) corporate sponsors for the meeting are:

SciVision

Internet Journal of Chemistry

Technical Sponsors are:

ACS CINF Division, ACS COMP Division, The Chemical Structure Association (CSA), Georgetown University - Department of Chemistry, Special Libraries Association (SLA) Chemistry Division, Royal Society of Chemistry (RSC)

17. Workshops at ChemInt2000

This note is to announce that three workshops have been arranged as part of the ChemInt2000 meeting program. These will be workshops by MDL, ACD, and SciVision. The ChemInt2000 meeting web Abstract Submission form is operational for the Chemistry and the Internet (ChemInt2000) meeting being held in at Georgetown University in Washington DC on September 23-26, 2000.

The draft program of invited speakers, workshops, markup language tutorial, and panel sessions (one on e-commerce chaired by Wendy Warr and one on Intranets and Internets chaired by Tom Pierce) is available on the meeting web site:

<http://www.chemint.org>

You are urged to look at the program and to consider submitting a poster paper to the meeting. Some 8-10 of poster papers will be selected for oral presentation at the meeting.

The main lecturers for the meeting will be:

Rene DePlanque (FIZ - Berlin), Jim Myers (Pacific Northwest Labs), Glen Hopkinson (Synopsys Scientific Systems), Wolf-Dietrich Ihlenfeldt (University of Erlangen-Nuremberg), Miloslav Nic (ICT Prague), Jim Ostell (NIH/NLM/NCBI), Engelbert Zass (ETH), Henry Rzepa (Imperial College, London), Peter Murray-Rust (Nottingham University)

18. Stereodynamics of Chemical Reactions

December 1 to 5, 2000

El Escorial (Madrid). SPAIN

Second Announcement

Format and Scope

This conference follows in scope and format the former meetings on Stereodynamics held in Jerusalem (1986), Bad Honnef (1988), Santa Cruz (1990), Assisi (1992), Gif sur Yvette (1994) and Bielefeld (1996).

The programme comprises invited lectures, posters and oral presentations in a spacious surrounding with ample time for discussion. The conference covers the field of reactive and non-reactive collisions involving atoms, molecules and surfaces of solids and liquids as well as half collisions. Major topics to be addressed are:

- * Stereocontrol of reactive collisions in the gas phase, on surfaces and in liquids.
- * Orientation effects in beam-surface reactions.
- * Brute force oriented molecules: collisions, spectroscopy, theory.
- * Effect of molecular orientation and alignment in non-reactive collisions.
- * Stereodynamics of photo-initiated reactions in Van der Waals complexes.
- * Collisions of orbitally aligned atoms.
- * In-situ measurements of orientation and alignment.
- * New Techniques.

General Information

Programme

Arrival is at 1st of December, departure at 5th of December. The scientific programme will consist of invited lectures (30 to 40 min in length), poster and oral presentations (20 min in length) of a few contributed papers. Social events will include a visit to the Monastery of El Escorial, a visit to the Prado Museum in Madrid, and the Conference Dinner.

Proceedings

The conference proceedings will be published in a special issue of a Scientific Journal. All manuscripts should represent new and unpublished work. The contributions will be reviewed in the normal manner. The abstracts of invited lectures and contributed papers will be collected in the book of abstracts. Copies of it will be distributed to the participants.

Registration fee

The Registration fee is 60.000 pts., including conference kit, full board, visit to the Prado Museum, visit to the Monastery and Conference Dinner. Registration fee may be paid from August, 2000 on, to the following account:

Branch: Caja de Madrid 2038 1735 91

Account N: 6000402693

Please send a copy of the bank transfer to:

Dr. Stefan Skowronek

Instituto Pluridisciplinar

Universidad Complutense of Madrid

Juan XXIII, 1

28040 Madrid

Conference fellowships are available upon request from Prof. A. Gonzalez Urea

Important Dates

* Payment and Registration 31st of August 2000

* Call for papers including further information and a list of invited speakers 30th of June 2000

Scientific Committee

R. Anderson (USA), V. Aquilanti (I), A. Gonzalez Urea (E), R.D. Levine (IL), H.J. Loesch (D), D. Parker (NL), J. Simons (UK), B. Soep (F), S. Stolte (NL), R. Vetter (F)

Local organisation

Angel Gonzalez Urea,

E-mail: stereody@eucmos.sim.ucm.es

Stefan Skowronek: Secretary of the Organising Committee.

Asuncin Garca Sousa: Secretary.

Address: Instituto Pluridisciplinar. Unidad de

Lseres y Haces Moleculares. P Juan XXIII-1. 28040-Madrid. SPAIN.

Fax: ++34.91.394 3265

19. New Frontiers in Chemical Reaction Dynamics

"New Frontiers in Chemical Reaction Dynamics" will be held at the Pacificchem Meeting next December (December 14-19) in Hawaii. The organizers of this symposium are: Hiroki Nakamura, George Schatz, Kopin Liu, Robert Continetti, and Toshinori Suzuki.

This symposium has been organized to discuss the present status and the future prospects of chemical reaction dynamics with the participation of both the theorists and experimentalists. Rapid progress that has been made in the understanding of the triatomic model reactions will be reviewed, and the new research directions toward complex multidimensional systems will be highlighted in the discussion and presentations. The topics will include:

- (i) dynamical stereochemistry (orbital alignment, steric effect, and vector correlations),
- (ii) dynamics involving multiple potential energy surfaces (interference effects, non-adiabatic transitions),
- (iii) multidimensional dynamics (reactions of tetraatomic system or larger, calculations of cumulative reaction probabilities, statistical and non-statistical nature of the dynamics),
- (iv) imaging chemical dynamics (transition state spectroscopy, ultrafast spectroscopy, multiparticle coincidence)
- (v) laser-control of molecular processes (including intense field dynamics).

Invited speakers (confirmed so far) are:

Neumark, Leone, Suits, Houston, Haydon, Miller, Truhlar, Skodje, Yarkony, Albert, Seideman, Lee, Yang, Mebel, Park, Smith, Kasai, Matsumi, Nagata, Kondow, Takatsuka, Aoyagi, and Takayanagi.

We welcome contributed presentations. Details of the meeting can be found at the ACS web page (www.acs.org) and in publications of the cosponsoring organizations in Japan, Canada, Taiwan, Australia, Korea.

20. Faraday Discussion No. 118: Cluster Dynamics

University of Durham, UK 18-20 April 2001

Studies of atomic and molecular clusters are one of the growth areas of modern chemical physics. The last few years have seen major advances in both experimental and theoretical methods, and it is now possible to prepare and characterize a wide range of finite-size systems.

Abstracts of papers containing new, unpublished work (not reviews) are invited for consideration by the Organising Committee. Summaries of about 300 words should be submitted no later than 31 March 2000 to Prof. Jeremy M Hutson, Department of Chemistry, University of Durham, Durham, DH1 3LE, UK (email J.M.Hutson@durham.ac.uk)

The Discussion will be focussed on studies that deal specifically with dynamical processes in a cluster environment and the interactions that determine them. The term "dynamics" will be interpreted widely, to include spectroscopic studies that probe multiple minima on a potential energy surface. The committee particularly welcomes papers in the following areas:

Reactions of clusters

Reactions induced by clustering

Transition-state spectroscopy

Photodynamics of clusters

Caging effects in clusters

Tunnelling in clusters

Global potential energy surfaces

ORGANISING COMMITTEE:

Professor Jeremy M. Hutson (Chairman) Professor Ad van der Avoird

Professor David C. Clary Professor Peter J. Knowles

Professor Klaus Mueller-Dethlefs Professor Anthony J. Stace

21. XIX INTERNATIONAL SYMPOSIUM ON MOLECULAR BEAMS

Università di Roma La Sapienza, June 4-8 2001

Following the tradition of the Molecular Beams meetings devoted to widespread applications of molecular beams coupled with electron, laser and synchrotron radiation, conference will be focused on dynamics of collisions, properties of clusters and methods of diagnostic.

Topics to be considered:

- Atomic and Molecular Spectroscopy
- Elementary Processes in Gas Phase
- Structure and Dynamics of Clusters
- Beam Surface Processing and Diagnostic
- Synchrotron Radiation Coupled with Molecular Beams

For informations, e-mail Professor Anna Giardini
e-mail: giardini@axrma.uniroma1.it

22. 26th International Symposium on Free Radicals.

"La Cittadella", Assisi, Italy, September 2-7, 2001.

Chairman: Piergiorgio Casavecchia (Universit di Perugia).

MARK YOUR CALENDAR!

A Web-page will become available at the beginning of the summer 2000.

Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, Universit di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy. E-mail: piero@dyn.unipg.it (Phone: (+39) 075 - 585 5514; FAX: (+39) 075 - 585 5606).

Special announcements

Chemical Kinetics and Photochemical Data for Stratospheric Modeling - Evaluation 13

This message is to announce the release of the volume, "Chemical Kinetics and Photochemical Data for Stratospheric Modeling - Evaluation 13", JPL Publication 00-3. This is the thirteenth in a series of evaluated sets of rate constants and photochemical parameters compiled by the NASA Panel for Data Evaluation. For the current release, the Panel has focused on a selected subset of the kinetic and photochemical parameters presented in the JPL 97-4 evaluation. JPL 00-3 updates and supplements JPL 97-4.

Evaluation 13 marks a change in approach adopted recently by the Panel. The scope of future releases will no longer include the entire database of stratospheric reactions and instead will focus on a few chemical families and/or topics in greater depth. It is expected that the entire database will be reviewed on a five-year cycle. Each evaluation, however, will include a section that addresses important reactions in any chemical family for which new work has been recently published.

Another significant change involves the format of publication. Evaluations will no longer be distributed in printed form. JPL 00-3 and JPL 97-4 are available for download in a variety of formats from the following Internet URL:

<http://jpldataeval.jpl.nasa.gov>

Requests for printed copies cannot be honored. For information on new releases, corrections, etc. subscribe to the email list as indicated on the web page.

We regret if you receive multiple copies of this message. Several different distribution lists have been used for this notification.

Stanley P. Sander Chair, NASA Panel on Data Evaluation

SPECIAL ISSUE European Physical Journal D

European Physical Journal D : Atoms, Molecules and Clusters (EPJ D)

SPECIAL ISSUE DEDICATED TO

"Femtosecond dynamics and coherent control in atoms, molecules and clusters: theory and experiment"

The understanding and control of the dynamics in atoms, molecules and clusters has been a tremendously growing field in the past decade. This has been acknowledged with the 1999 Nobel prize in chemistry awarded to Ahmed Zewail.

The purpose of this issue is to collect the newest results in the field of ultrafast dynamics and coherent control in the gas phase. The subfields we want to cover include theoretical and/or experimental studies of

- ultrashort dynamics in atoms, molecules and clusters,
- atoms, molecules and clusters in strong laser fields : ATI, ATD, Coulomb explosion ..., and control of such processes
- coherent control and/or optimal control of ultrafast dynamics, using short or shaped laser pulses,
- coherent control schemes based on quantum interference between excitation paths,
- coherent control schemes based on a subtle manipulation of the internal quantum state, such as Rapid adiabatic passage, "pi" pulses...

Thus an up-to-date overview of this exciting and vastly developing area will be provided.

Authors are encouraged to submit original research papers containing experimental and/or theoretical work to the guest editors :

Pr Bertrand GIRARD

Université Paul Sabatier, Toulouse III

Laboratoire Collisions, Agrégats, Réactivité

IRSAMC UMR 5589

118 Route de Narbonne

31062 Toulouse cedex FRANCE

Tel. : (33) 5 61 55 64 98

Fax : (33) 5 61 55 83 17

bertrand@yosemite.ups-tlse.fr

Pr. Volker Engel

Institut für Physikalische Chemie

Universität Würzburg

Am Hubland

D-97074 Würzburg

Tel.: +49-931-888-6376 (office)

Fax : +49-931-888-6378 (fax)

E-mail voen@phys-chemie.uni-wuerzburg.de

Alternatively, submissions can be made to the EPJ editorial office in Orsay, with the clear statement of the Special Issue. All submissions will be reviewed in accordance with the normal review procedures of the journal.

Deadline for submission is Sep. 1st 2000. Manuscript arriving after this date cannot be considered for publication in the special issue.

Authors willing to contribute are kindly asked to inform the editors and give a (tentative) title until June, 1st.

Organization: FIZ CHEMIE BERLIN

What are "ChemGuides"? These are a specific type of Internet database/information system which is specialised in locating chemistry-relevant Web sites.

Try our ChemGuides and their extremely powerful search options. Why don't you just check to see where we have found you and at the same time test the systems' performance?

The ChemGuides are accessible via our Web Site:

<http://www.chemistry.de/>

or directly at

<http://www.chemistry.de/en/datenbanken/chemguide/>

And when you are already logged on, perhaps you might also like to try our free "PublishersGuide - Science and Technology", which covers the Internet pages of scientific publishers and is also available via our Web site.

<http://www.fiz-chemie.de/en/datenbanken/publishersguide/>

BOOKS and SOFTWARE

Program announcement

"MULTIMODE"; a code to obtain accurate rovibrational energy levels for many-mode molecules by: S. Carter, 39, Grove Hill, Caversham, Reading RG4 8PS, UK J.M. Bowman, Department of Chemistry, Emory University, Atlanta GA 30322, USA and contributions from N.C. Handy, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW, UK

"MULTIMODE" is a near-variational procedure for the calculation of rovibrational energies of polyatomic molecules, adsorbates and clusters.

The method is based on the Watson normal coordinate hamiltonian for non-linear molecules, and proceeds via vibrational SCF and rovibrational CI steps. The complete hamiltonian is used at all times, but approximations are made in order to integrate the potential and coriolis terms. These terms are included as N-mode expansions in the normal coordinates, but are truncated at the 4-mode terms. It has been demonstrated that higher terms are insignificant compared with the inaccuracies in the potential itself. The method has been thoroughly tested for a variety of triatomic and tetraatomic molecules and, in particular, against exact variational results for H₂CS (6 modes, ref. 1) and more recently it has been applied to CH₄ (9 modes, ref. 2). In both cases, excellent convergence has been achieved for all of the low-lying vibrational levels.

"MULTIMODE" can be used in less accurate calculations, for example at the SCF level alone, or in SCF-CI calculations, where specified numbers of vibrational (non-orthogonal) SCF functions are used in a vibrational CI basis. These methods also allow for an adiabatic rotation scheme, which gives reasonable values for rotational constants, in particular.

"MULTIMODE" is currently being extended to include the Watson hamiltonian for linear molecules, and also to include the Miller-Adams-Handy Reaction Path hamiltonian in order to describe a single large-amplitude coordinate, for example the torsion in H₂O₂. This will widen the scope of molecules that can be handled.

information:

www.emory.edu/CHEMISTRY/faculty/bowman/multimode

enquiries:

s.carter@reading.ac.uk

References ———

1. S. Carter, J.M. Bowman and N.C.Handy; Theor. Chem. Accts., 100, 191 (1998)
2. S. Carter and J.M. Bowman; J. Phys. Chem. 104, 2443 (2000)