

Molecular Dynamics News

number 108; August 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 has been accepted - otherwise state *unpublished*).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 109 to Prof. V. Aquilanti. (We greatly appreciate that you use electronic mail because our editorial resources are very limited: AQUILA@DYN.UNIPG.IT). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#108). The closing date for issue number 109 is October 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**

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ELECTRONIC DELIVERY OF MDN

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

1. Electronic mail to subscribers

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

2. World Wide Web

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

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

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

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

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

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

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

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

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

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

In Memorial

The Molecular Dynamics community is greatly saddened by the recent death of Kent Wilson, and we reprint the following story about Kent with the kind permission of Kim McDonald (<http://ucsdnews.ucsd.edu/newsrel/science/mcwilson.htm>) so that our readers may be reminded of the remarkable achievements of Kent.

RENOWNED UCSD CHEMISTRY AND BIOCHEMISTRY PROFESSOR KENT R. WILSON DIES ON MARCH 27

Known internationally for his achievements in the molecular dynamics of chemical and biochemical reactions, Professor Wilson was a prominent member of UCSD's faculty who dreamed of uncovering the most exquisite details of chemical reactions and of building the best chemistry department in the world.

"He was a beloved and respected member of the department, the university and the international scientific community," said Katja Lindenberg, a professor of chemistry and biochemistry at UCSD. "Kent touched and enriched many lives and will be sorely missed. His indelible personal and professional mark will long remain stamped on everyone who had the privilege of knowing him."

Professor Wilson's thirst for discovery and new frontiers led to many firsts that have endured the test of time as important contributions in several areas of chemistry. In the late 1960s, he and his research group developed the technique of photofragment spectroscopy that enabled them to probe the unstable states of molecules. In the 1970s, he used laser spectroscopy to unveil the chemistry of atmospheric pollution. In the 1980s, he combined ultrafast laser experiments with computer simulations to develop an understanding of how reactions occur in solution. In the past decade, he led a very ambitious effort to use ultrafast beams of x-rays to probe and control chemistry. The techniques developed by Professor Wilson have had widespread application in fields as diverse as atmospheric pollution, ancient statue dating, chemical reactions in liquids, and the development of pulsed x-ray sources and laser microscopes for use in sophisticated analysis of biological systems.

He was raised in a mostly Quaker community in Bryn Gweled Homesteads, Penn., and his decision to become a scientist was inspired by prominent scientists in his community, by his own mischievous childhood experiments, such as rewiring the town's phone system, and by disassembling and repairing household appliances. His particular interest in chemistry began through a high school fascination with moonshine and fireworks, which he made using surplus World War II equipment.

Professor Wilson received his bachelor's degree in chemistry and physics from Harvard University in 1958 and completed his doctorate in 1964 under the guidance of Harvard Nobel Laureate Dudley Herschbach at the University of California, Berkeley. He shared a lab with a group of graduate students who would all become fellow pioneer laser spectroscopists: Dick Zare, Jim Kinsey, and Yuan Lee. After postdoctoral work at Harvard and the National Bureau of Standards, he joined the UCSD faculty in 1965.

According to members of his department, Wilson brought a love of exploration and learning to his life as a faculty member: He loved the freedom it gave him to be an adventurer and a buccaneer, to explore the unknown, to follow his own unquenchable hunger for knowledge, and to educate and inspire young minds.

He was also one of the most innovative teachers at UCSD. For 30 years, he pioneered the use of visualization technologies to make science more accessible to students of all ages. Many students and postdoctoral researchers at UCSD remember watching Professor Wilson's films in high school. He brought films and other visualization techniques to the classroom when these technologies were in their infancy. Instead of employing professional programmers in this effort, he relied on a hand-picked team of some of the brightest undergraduate students he brought together in a group he dubbed the Senses Bureau. This group of extraordinarily talented undergraduates focused on the multisensual use of computer visualization, sound and touch as tools in research and education. The students did some of the original work on what is now called "virtual reality," and designed and created computer animations that have enhanced the visualization of scientific concepts in the classroom. Some of these students passed up other opportunities and specifically came to UCSD because of his legendary invitation, their first opportunity to experience his formidable

talents in the art of persuasion and negotiation.

Professor Wilson's approach to research was unique: He felt that the first key to success in difficult experiments was to search the world for the best young scientists to work in his laboratory. He believed that the second, and perhaps most important, key to success was to facilitate teamwork among his brilliant junior collaborators. He was so proud of his international research team in the 1990s that he referred to them as his Dream Team, alluding to the highly successful U.S. Olympic basketball squad.

Professor Wilson received numerous distinctions during his prolific career. He was a Fellow of the American Physical Society and of the American Association for the Advancement of Science. Perhaps his most enduring legacy lies in the large number of his students and junior associates that went on to outstanding careers and achievements of their own all around the world. His life ended during one of the most productive and exciting periods of his career, which was evidenced by his many publications, especially the recently published work in the journals *Science* and *Nature*. His scientific work at UCSD will be continued under the direction of Jeff Squier.

In addition to his passion for science, Professor Wilson was instrumental in preserving large portions of Torrey Pines State Park. He shared a love of bodysurfing in the Pacific with his daughter Tasha and a love of books and music with his daughter Maya. Kent Wilson is survived by his wife of 32 years, Lana Wilson, a potter. He is also survived by two daughters, Tasha Wilson, a clinical social worker, and Maya Wilson Chakko, a public policy analyst; and his son-in-law, Matthai Chakko, all of whom live in Northern California.

a. Open Positions

FACULTY

PERMANENT RESEARCH STAFF POSITION, IAMS, TAIWAN

The IAMS of Academia Sinica in Taiwan invites applications for a tenure-track position at the level of assistant research fellow in experimental chemical dynamics. Applicants should have a Ph.D. in chemistry or physics and an excellent track record in research in the general area of gas phase physical chemistry or chemical physics. Two years postdoctoral experience is desirable. The initial appointment will be for four years in collaboration with Dr. Kopin Liu at IAMS. The successful candidate is anticipated to establish his/her own research program upon promotion. The IAMS is rapidly developing into one of the world's prime research institutions, offering excellent working conditions and technical support. Additional information can be glanced at <http://kliu.iams.sinica.edu.tw/>. Applications with three letters of recommendation, full curriculum vitae including 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

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:

1 for 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

1 for 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.

1 for 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

Or please fax to: Professor and Vice Director Gao, Zhen at 86-010-62563167

Or please mail to: Professor & Director Gao, Zhen

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/>

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, UNIVERSITY OF MONTREAL

Owing to the decision of an applicant to withdraw, a postdoctoral position is again 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), JCP 112 8765 (2000));

(ii) rate constants (Chem Phys Lett 267 417 (1997), Chem Phys Lett 293 209 (1998)),

(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,

POSTDOCTORAL POSITION, 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 POSITION, UNIVERSITY OF WATERLOO

I have PDF openings in experimental projects involving spectroscopy of atmospheric species.

The projects relate to the increasingly important area of the chemical identification of atmospheric species by remote sensing methods. They include both field measurements and laboratory studies. The duties require some familiarity with laser spectroscopy and FTIR.

For more information, please see:

<http://sciborg.uwaterloo.ca/~sloanj/grad.html>

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

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

POSTDOCTORAL POSITION, UNIVERSITY OF INDIANA

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

POSTDOCTORAL POSITION, COMPLUTENSE UNIVERSITY, MADRID

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 July 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 POSITION, BEN-GURION UNIVERSITY

A post-doctoral position is available at Ben-Gurion University with Professor Yehuda Band to carry out research on ultra-cold atom collisions, Bose-Einstein condensation, coherent matter waves, quantum information and quantum computing, nonlinear optics and optical pulse propagation in dispersive media. Candidates should be familiar with collision theory, close-coupling methods, molecular physics, and/or linear and nonlinear optics, and have experience in fortran programming.

In order to apply, send CV and arrange for two letters of recommendation to be sent to:

Professor Yehuda Band, Departments of Chemistry and Physics, Ben-Gurion University, Beer Sheva, 84105 ISRAEL

The approximate starting date for the position is September/October.

For further information contact Yehuda Band at E-Mail Address: band@bgumail.bgu.ac.il

Address, telephone and FAX abroad (until September): Professor Yehuda Band, National Institute of Standards and Technology, 100 Bureau Drive Stop 8423, Gaithersburg, MD 20899-8423

Phone: 301-975-8561, Fax: 301-990-1350,

POSTDOCTORAL POSITION, WAYNE STATE UNIVERSITY A 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 dynamics 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. The high-performance computing architecture available for this research includes a 24 processor IBM-SP and a 54 processor SUN cluster. Please contact William L. Hase, Department of Chemistry, Wayne State University, Detroit, MI 48202, USA; email wlh@chem.wayne.edu. Wayne State University is an equal opportunity employer.

POSTDOCTORAL POSITION, HEBREW UNIVERSITY OF JERUSALEM

I wish to advertise two positions which are offered either at the Ph.D. or post-doc level, concerning applications of ultrafast spectroscopy to chemical dynamics in condensed phases. The research will be conducted in the physical chemistry department at the Hebrew University in Jerusalem, Israel. The first project deals with developing novel pulse shaping and multichannel optical detection techniques for implementation of control schemes in condensed systems. The other will address primary light induced events in native and synthetically modified bacteriorhodopsins. The laboratory provides a wide base of state of the art equipment, including 2 amplified 30 fsec laser systems, an OPA producing ~20 fsec pulses, THz generation and detection equipment, and multichannel as well as single frequency detection systems for pump-probe spectroscopy. Preference will be given to candidates who have prior experience with ultrafast lasers. Interested parties are encouraged to contact me for further details, and are requested to provide letters of reference from people who are closely acquainted with their work.

Sanford Ruhman

POSTDOCTORAL POSITION, JILA, UNIVERSITY OF COLORADO

A postdoc position is available beginning immediately in the group of John Bohn at JILA. The project will center on the theory of ultracold molecular gases, including cold collisions, novel types of ultracold chemistry, and possibilities for new phenomena in Bose-Einstein condensates. Candidates with a background in scattering theory, molecular physics, theoretical chemistry, or many-body physics are particularly encouraged to apply.

JILA is an interdisciplinary institute located in beautiful Boulder, Colorado at the foot of the Rocky

Mountains. For details on JILA postdoc positions, including the application form, please visit the "Research and Job Opportunities" section of the JILA website, <http://jilawww.colorado.edu/> . Also feel free to contact me at bohn@murphy.colorado.edu for further information on this position.

John L. Bohn, Associate Fellow, JILA, Research Assistant Professor, University of Colorado, JILA, Campus Box 440, University of Colorado, Boulder, CO 80309

Phone: (303) 492-5426, Email: bohn@murphy.colorado.edu , URL: <http://condon.Colorado.EDU/~bohn/>

POSTDOCTORAL POSITION, UNIVERSITY OF YORK

An EPSRC-funded postdoctoral research assistantship is available from October 1 2000 for 3 years. The research will involve development of time-resolved infrared spectroscopy and its applications to laser photochemistry of organometallics. The research programme is led by Professor Robin Perutz and Dr Simon Duckett. Their research groups have an international impact and strong links with other groups in Europe and North America. Candidates should have extensive experience of laser spectroscopy. Salary will be in the range from 16755 to 18737. For information about the University and the research, consult the World Wide Web at <http://www.york.ac.uk> and <http://www.york.ac.uk/depts/chem/staff/rnp> respectively. Candidates are asked to submit three copies of a full curriculum vitae, together with the names of two referees to the Director of Personnel, University of York, York YO10 5DD, UK, from whom further information may be obtained. Closing date Aug 25 2000. For informal inquiries contact Professor Perutz (tel +44-(0)1904-432549, e-mail rnp1@york.ac.uk).

POSTDOCTORAL POSITION, UNIVERSITY OF WATERLOO

The position is available immediately. It involves the development of new laser and FTIR spectroscopic instruments for applications in remote sensing of tropospheric aerosols. Candidates should have some experience with lasers and spectroscopy, and also should have some scientific programming skills. The project is supported by the Centre of Excellence for Earth and Space technology and by the Canadian Space Agency. Two industrial partners are participating in the instrument design. Validation and testing is being done in collaboration with scientists from Environment Canada and the Ontario Ministry of the Environment, and involves field studies organized by both agencies. The candidate will have the opportunity to work with atmospheric scientists in these laboratories, and will interact extensively with our industrial partners.

General information about other current projects in our laboratory may be found at:

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

The University of Waterloo is located about 100 km west of Toronto, in a pleasant, rural setting. It has approximately 20,000 students. The Kitchener-Waterloo urban area has a population of approximately 250,000. The position is for one year initially, extendable subject to mutual agreement and the availability of funds. Applicants should forward a CV and two letters of reference to:

Prof. J.J. Sloan, Department of Chemistry, University of Waterloo, Waterloo ON N2L 3G1 Canada.

Fax: 1 519 746 0435, e-mail: sloanj@UWaterloo.CA

POSTDOCTORAL POSITION, UNIVERSITY OF ECOLE NORMALE SUPERIEURE, PARIS

A postdoctoral position in femtosecond physical chemistry is open at the department of chemistry of Ecole Normale Supérieure (ENS) of Paris, in the CNRS unit 8640. The research project deals with photoinduced elementary processes in organic materials and biological photoreceptors in condensed phase, studied by time-resolved femtosecond UV-visible absorption spectroscopy. The project involves the development of a pump-probe set-up with sub-50 fs time-resolution by using an amplified Ti:Sapphire laser and a visible OPA. Two 500-fs dye-laser systems and a pump-probe set-up are presently available for absorption and gain spectroscopy with subpicosecond resolution, in addition to a streak camera for time-resolved fluorescence. This research will be developed in a group involving three permanent researchers, in a collaborative effort with other ENS groups in synthesis and theoretical chemistry.

ENS is located downtown Paris in the Latin district. The position is for one year, starting between October and December 2000. The applicant should not be from the European Community but from any other* of the 29 countries of OECD plus Brazil, China and India. He/She should be less than 35 years old. The salary is

12000FF (1829 Euros) per month plus health insurance for the applicant. Experience in femtosecond time-resolved spectroscopy will be considered. Applicants should send their CV and three letters of recommendation to the address below.

*(Australia, Canada, Czech Republic, Hungary, Iceland, Ireland, Japan, Korea, Mexico, New Zealand, Norway, Poland, Switzerland, Turkey, USA)

Monique Martin, Director of Research, UMR ENS-CNRS 8640, PASTEUR, Departement de Chimie, Ecole Normale Superieure, 75231 Paris Cedex 05 - France

Phone: 00 33 (0)1 44 32 24 12, Fax: 00 33 (0)1 44 32 33 25, email: Monique.Martin@ens.fr

POSTDOCTORAL POSITION, ARGONNE NATIONAL LABORATORY

A postdoctoral or visiting scholar position is available in the Chemistry Division of the Argonne National Laboratory in the area of theoretical and computational studies of atomic clusters and nanoparticles. The studies cover a broad variety of physical and chemical properties of these systems and related phenomena, including interactions with molecules and substrates. Both, homogeneous and heterogeneous, e.g., alloy, systems are considered. The work involves general analytical and methodological developments especially relevant for the finite size regime, code development, and large-scale computer simulations. Excellent computational resources are available. Highly motivated, creative, and desiring to excel candidates with background in quantum chemistry, theoretical chemistry and/or solid state physics, classical and quantum dynamics, and related fields are welcome to apply. Argonne offers highly competitive compensation and excellent benefits. The appointment is initially for one year with a possible extension upon mutual agreement. Interested candidates should forward their CV and list of publications and arrange for three recommendation letters to be sent to

Dr. Julius Jellinek, Chemistry Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

E-mail: jellinek@anlchm.chm.anl.gov , Tel.: (630)252-4729 , FAX: (630)252-4954

POSTDOCTORAL POSITION, GENESIS RESEARCH INSTITUTE, EAST TOKYO

Postdoctoral Position, Genesis Research Institute, Inc. in collaboration with Cluster Research Laboratory, Toyota Technological Institute A postdoctoral position is now available in the laboratory of Tamotsu Kondow in East Tokyo Laboratory of Genesis Research Institute, Inc. and Cluster Research Laboratory of Toyota Technological Institute. The postdoctoral fellow will work on cluster deposition onto a solid surface at a pressure as low as 10⁻¹⁰ Torr and observation of a deposited cluster by using STM operated at 6 K and 7 T, together with optical probes, which will be available. The initial appointment will be for one year, with possible renewal for the second year. Salary will be competitive, and the position includes excellent health insurance. If interested, please send a CV, one reprint for each paper, and arrange for two letters of recommendation to be sent: Tamotsu Kondow, Professor of Cluster Research Laboratory, Toyota Technological Institute: in East Tokyo Laboratory, Genesis Research Institute, Inc. Futamata 717-86, Ichikawa, Chiba 272-0001, Japan. Phone: +81-47-320-5911, FAX: +81-47-327-8031, E-mail: kondow@mail.cluster-unet.ocn.ne.jp , WWW: <http://www.cluster-unet.ocn.ne.jp>

POSTDOCTORAL POSITION, UNIVERSITY OF SOUTHERN CALIFORNIA

A postdoctoral position is available in the laboratory of Professor Steve Bradfort 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 Bradfort, 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/>

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

POSTDOCTORAL POSITION, UNIVERSITY OF UTAH

A post-doctoral position is available immediately in the field of soft condensed matter simulations in the Department of Materials Science and Engineering at the University of Utah. Candidates should have a strong background in molecular dynamics simulations of molecular liquids, solutions, liquid crystals and/or polymers.

The position provides opportunities to work on a variety of projects, including property prediction for the ASCI Center for the Simulation of Accidental Fires and Explosions (<http://www.csafe.utah.edu/>), simulation of aqueous polymer solutions and hydrogels, simulations of ionomers and polyelectrolytes and simulations of polymer structural materials and nanocomposites. In addition to simulations, responsibilities will include model and algorithm development and implementation, project management, and student supervision. The position also provides extensive opportunity for close collaboration with experimentalists. Information regarding our group can be found at <http://www.che.utah.edu/~gdsmit/>. Interested parties should send their resume to Grant Smith at gsmith2@geoffrey.emro.utah.edu

POSTDOCTORAL POSITION, UNIVERSITY OF LEIDEN INSTITUTE OF CHEMISTRY

A postdoc position is available in a joint project of the Theory Group of the Leiden Institute of Chemistry (Dr. M.C. van Hemert) and the Molecular Astrophysics Group at the Leiden Observatory (Prof. Dr. E.F. van Dishoeck).

The project involves the study of dissociative recombination, a basic chemical process which occurs in a wide variety of plasmas, but which at present is not well understood for even the simplest systems. Molecules for which dissociative recombination will be investigated are astrophysically and/or atmospherically important polyatomic ions, in particular CH_2^+ , H_2O^+ and H_3O^+ . A high level ab initio (Multi-Reference Configuration Interaction or MRCI) method will be used to obtain the potential energy surfaces of the ion and of the neutral molecule which dissociates after the capture of the electron. The nuclear motion towards dissociation on these surfaces will be followed with wave packet dynamics, taking into account non-adiabatic couplings between these surfaces when necessary (also obtained with MRCI). Innovative aspects of the project include the modeling of the initial state (the molecular cation + the electron to be captured) and the calculation of the manifold of highly excited Rydberg states. The results will be compared with new experiments and will provide insight into the basic mechanism for single vs multiple bond breaking.

The position is available starting anytime after 15 September 2000, for a total period of two years. Scientists with a Ph.D. in Chemistry, Physics, or numerical Mathematics who are interested in molecular quantum mechanics and have experience with numerical methods and computer programming are asked to apply. The total salary (before taxes) will be between dfl 5153,- and dfl 8682,- per month, depending on experience.

If interested, please send a letter and CV by airmail to the below address, and arrange for two letters of recommendation, to be sent as well to the below address (please use ordinary or air mail, not e-mail). The deadline for receiving letter and CV is 1 September 2000

M.C. van Hemert (mvhemert@chem.leidenuniv.nl), LIC, Gorlaeus Laboratoria, Rijksuniversiteit Leiden, Postbus 9502, 2300 RA Leiden, The Netherlands
(Tel +31 71 527 4244, Fax +31 71 527 4488)

Information on the theory group can be found on rulgla.leidenuniv.nl Information on the molecular astrophysics group is in <http://www.strw.leidenuniv.nl/astrochem>

POSTDOCTORAL POSITION, SRI INTERNATIONAL

The Physics and Atmospheric Chemistry (PAC) Unit of the Molecular Physics Laboratory (MPL) is searching for well-qualified candidates for a post-doctoral position in experimental physical chemistry. The work involves collision energy transfer studies of excited states of molecular nitrogen, typically by means of pump-and-probe ionization techniques, under the supervision of Professor Marshall Ginter of the University of Maryland working in the laboratories of Dr. Richard Copeland at SRI International. These studies are

directed towards an improved understanding of upper atmosphere processes. Electronically excited nitrogen molecules are an important species in the upper atmospheres of Earth and are to be investigated as part of a program to study auroral processes.

SRI International is a nonprofit contract research organization, located in Menlo Park, California, in the San Francisco Bay region, and is one of the largest such establishments in the world. Many areas of research are represented by the investigations carried out at SRI, including chemistry, physics, engineering, life sciences, computer sciences, education, and a variety of other disciplines. MPL has an international reputation for creative and innovative research in atmospheric studies, combustion processes, surface science, plasma research, and molecular beam research. Within MPL, the members of the PAC unit have been active for many years in studying the chemistry and physics of the atmosphere, with Dr Copeland's emphasis on the processes that occur in the 80-120 km night airglow region. There has been close coupling between the laboratory kinetics studies that this group carries out, and the results of optical emission studies by field observers.

The postdoctoral assistant will be employed by the University of Maryland and will perform the experiments at SRI International as a visiting scientist. We expect the candidate to have experience in the operation and maintenance of pulsed laser systems. Other qualifications include a Ph.D. degree in chemistry or physics, and beyond laboratory abilities, effective technical writing is an important attribute for the position, as well as an ability to make oral presentations. Appointment is for a minimum of one year, with a second year normally being available upon mutual agreement.

A resume, three letters of recommendation, and a one page "research interests" summary should be sent to: Dr. Richard A. Copeland, PS091, Molecular Physics Laboratory, SRI International, Menlo Park, California 94025

Telephone: (650) 859-6534, email: richard.copeland@sri.com

POSTDOCTORAL POSITION, LAWRENCE BERKELEY NATIONAL LABORATORY

We have an opening for a post-doctoral fellow at the Chemical Dynamics Beamline of the Advanced Light Source in Berkeley, CA. Please alert potential candidates about this opportunity. There are currently 9 beamline scientists working at three different end-stations on a variety of projects from spectroscopy to dynamics.

PROJECT DESCRIPTION: The project involves experimental studies of radical photochemistry and crossed-beam reaction dynamics; flame diagnostics, the development of new radical molecular beam sources; innovative applications of synchrotron radiation to chemical dynamics studies such as coincidence imaging of photochemical products. Some of the work will be carried out in collaboration with outside users.

QUALIFICATIONS: PhD (within last four years) in Chemical Physics or a related discipline, experience in molecular beam photochemistry or reaction dynamics studies and a record of publication in chemical dynamics, spectroscopy, or a closely related field.

STARTING DATE: Anytime after September 1, 2000

Research will be jointly supervised by Tomas Baer and Dan Neumark

Send resume and at least 2 letters of recommendation to: Tomas Baer at tbaer@lbl.gov, or

Tomas Baer, Chemical Dynamics Beamline, ALS, Lawrence Berkeley National Laboratory, 1 Cyclotron Road; Mailstop 2-6100, Berkeley, CA 94720

<http://www.lbl.gov/chemicaldynamics/>

POSTDOCTORAL POSITION, UNIVERSITY OF SURREY

A 3-year EPSRC-funded postdoctoral research assistantship is available from October 1 2000 for work with Dr Peter B Karadakov and Prof Graham A Webb on the development and applications of new ab initio methodology and computer codes for the calculation of NMR shielding tensors in extended one-, two-, and three-dimensional systems with translational symmetry.

Applicants should have a PhD in theoretical chemistry or chemical physics and good programming skills in FORTRAN. Previous experience with ab initio codes such as GAUSSIAN and CRYSTAL is highly desirable.

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

Further information can be obtained from:

Dr Peter B Karadakov (e-mail: p.karadakov@surrey.ac.uk) or Prof Graham A Webb (e-mail: g.webb@surrey.ac.uk)

Applications should be accompanied by a CV and the names and addresses of two referees. Closing date September 30 2000.

POSTDOCTORAL POSITION, UNIVERSITY OF MANCHESTER

Fundamental Molecular Beam Studies of Atom, Radical, Ion-Induced Reactions in Plasma-Surface Interactions.

This project is funded by the UK Engineering and Physical Sciences Research Council under its Technological Plasma Initiative. The aim of the project is to study the reactions of atoms, molecular, radicals and ions with semiconductor III-V surfaces important in plasma etching. An existing crossed-molecular beam apparatus will be modified to provide a unique experimental facility for the study of fundamental processes occurring in plasma-surface reactions.

These experiments follow on from existing studies of the gas-surface chemistry involved in the reactive plasma etching of III-V semiconductors using time-of-flight mass spectroscopy and laser-induced fluorescence. The Plasma Chemistry group at Manchester is also involved in research into a variety of plasma-based, environmental clean-up procedures for pollutants in gaseous waste streams including VOC's and diesel exhausts. A strong emphasis is placed on understanding the chemistry of the processing in order to better optimise the process and considerable effort goes into the development of computer-based kinetic models.

Applications are invited from Ph.D. scientists with experience in molecular beam-surface scattering, time-of-flight mass spectroscopy and laser spectroscopy. The position will be available from 1st October 2000. The appointment will be for up to two years at a salary in the range 16,286 - 18,185, p.a. (under review), according to age and experience.

Informal contacts may be made of either Dr P.A. Gorry (p.a.gorry@man.ac.uk; +44 0161 275 4676) or Dr J.C. Whitehead (j.c.whitehead@man.ac.uk; +44 161 275 4692) or by mail at Chemistry Department, Manchester University, Manchester M13 9PL, U.K.

Applications should be made on a form provided by the Personnel Department (personnel@man.ac.uk) quoting the Reference Number (594/00). Applicants should also arrange for two or three academic referees to send references directly to Dr Gorry or Dr Whitehead. The deadline for applications is 15th August 2000. Details of Manchester University, the Chemistry Department and of Manchester and its environs can be found on the web site <http://www.man.ac.uk/>

POSTDOCTORAL POSITIONS, EMORY UNIVERSITY

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

The fellows will be involved in

Theoretical studies of structures and reactions of transition metal complexes, such as bioinorganic systems, organometallic compounds and homogeneous catalysts,

or Development of the ONIOM (Our own N-layered Integrated molecular Orbital + molecular Mechanics) method and computer code and its applications. (A good knowledge of the Gaussian code is essential for this project.)

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

The position can start immediately or by spring 2000. The appointment is originally for one year, but an extension to the second year is possible with mutual agreement.

This fall we will be moving into the top floor of the new Cherry Logan Emerson Building, and will upgrade the Emerson Center computing facilities.

Keiji Morokuma, William H. Emerson Professor of Chemistry, Department of Chemistry, Director, Cherry L. Emerson Center for Scientific Computation, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, USA
Phone (404) 727-2180; Fax (404) 727-6586, E-mail: morokuma@emory.edu, Web:
<http://euch4m.chem.emory.edu>

POSTDOCTORAL POSITION, UNIVERSITY COLLEGE LONDON

A postdoctoral position is available in the Chemistry Department at UCL to study the formation, reactivity and decay of molecular dipositive ions (dications) using both experimental and theoretical techniques. The position, which is available immediately, is for one year in the first instance with the possibility of renewal for an additional 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. Other nodes of the network are in Trento (Italy), Berlin (Germany), Prague (Czech Republic), Innsbruck (Austria), Perugia (Italy) and Wein (Austria). Funding is available for the successful applicant to spend some time at several of the above locations in addition to UCL..

The project will be supervised by Dr Stephen D. Price and Dr Nikolas Kaltsoyannis. Further information on the studies of molecular dications performed at UCL can be obtained from the UCL chemistry web server:
<http://www.chem.ucl.ac.uk/people/sdprice/index.html> <http://www.chem.ucl.ac.uk/people/nkalt/index.html>
Additional 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 to either Dr Stephen D. Price or Dr Nikolas Kaltsoyannis at Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ. UK

POSTDOCTORAL POSITION, UNIVERSITY OF SUSSEX

Applications are invited for a postdoctoral fellowship to develop cooling and trapping techniques of molecules with specific applications to molecular radicals. This position will be in the group of Professor E. A. Hinds at the Sussex Centre for Optical and Atomic Physics and is funded by PPARC, as part of the "Measurement of the Electric Dipole Moment of the Electron" project.

The projects to be developed in our laboratory are concerned with creating a source of molecular radicals (YbF and BaF in particular), translationally and internally cooling the molecules that are formed and performing high resolution spectroscopic measurements upon them.

This position would particularly suit a recently-graduated chemical physicist or physical chemist who has a strong interest in the manipulation and trapping of molecules and considerable experience with some of the following: lasers, molecular beams, resonance enhanced multiphoton ionisation (REMPI) or time-of-flight mass spectrometry (TOFMS). Good oral and written presentation skills and the ability to work amiably in a group are absolutely essential.

The position (for up to 3 years duration) is available from Sep 2000 although the exact start date is negotiable. There are no nationality requirements for this position.

For further information about the position, please contact Prof. E. A. Hinds, SCOAP, CPES, University of Sussex,

(01273) 678081, (01273) 677196, e.a.hinds@sussex.ac.uk

<http://pburton.maps.susx.ac.uk/scoap/index.html>

POSTDOCTORAL POSITIONS, UNIVERSITY OF PERUGIA

POSTDOCTORAL POSITION (a)

Applications are invited for a postdoctoral position under the supervision of Professor Piergiorgio Casavecchia, and funded by the European Union's TMR (Training and Mobility of Researchers) Programme, as part of the TMR Network on "Astrophysical Chemistry: Experiments, Calculations, and Astrophysical Consequences of Reactions at Low Temperatures". This programme involves eight laboratories: University of Birmingham (UK), University College London (UK), University of Goettingen (Germany), Technische Universitat Chemnitz (Germany), University of Rennes (France), Observatoire de Paris, Meudon (France), University of Bordeaux (France), and the University of Perugia (Italy). The focus in our laboratory is on studies of chemical reaction dynamics using the Crossed Molecular Beams scattering technique with universal mass-spectrometric detection. Investigation of elementary atom(radical)-molecule and atom-radical reactions of relevance to Astrochemistry are being pursued. We exploit the novel capability of generating intense and continuous supersonic beams of carbon and nitrogen atoms, and hydroxyl (OH) and cyano (CN) radicals. All these beams have already been successfully tested and used for experiments. Experiments are planned on N, C, and CN reactions, as well as on atom-radical reactions as N+OH. More details of the research field, the technique used, and publications may be found at the following site: <http://www.chm.unipg.it/chimgen/mb/exp3/casavecchia.html>

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

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

The position is available from November 1st, 2000 for one year (actually 13 months). The exact commencement date is negotiable. The post-doc is expected to spend up to one month each year in another laboratory of the TMR network. Salary is about 3000 EURO/month. Under the terms of the TMR Programme, applicants must be nationals of a Community Member State or a State associated with the TMR Programme (Iceland, Israel, Liechtenstein, Norway). The young researchers must not be nationals of the state in which the participant appointing them is established (i.e., Italy) and must not have carried out their normal activities in that state for more than 18 of the 24 months prior to their appointment. Experience in reaction dynamics and molecular beams is desirable. Interested candidates should send a Curriculum Vitae to the address below using conventional or electronic mail. The name and addresses of two referees should also be provided at this time. Informal inquiries are also welcomed. Prof. Piergiorgio Casavecchia, Dipartimento di Chimica, 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).

POSTDOCTORAL POSITION (b) at DEPARTMENT OF CHEMISTRY - 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/chimngen/mb/exp3/casavecchia.html>

and details of the REACTION DYNAMICS Network should also be consulted:

http://www.chm.unipg.it/chimngen/Reaction_Dynamics.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).

POSTDOCTORAL POSITIONS, KTH, STOCKHOLM

Accelerator driven transmutation of nuclear waste is not only one of the fastest growing fields in modern science, but also one of the most rewarding! Hereby we announce two opportunities to participate in a work that makes people write to their governments and nobel prize laureates rotate in their graves!

The department of Nuclear and Reactor Physics at KTH participates in the EU 5th Framework Program on nuclear waste transmutation. Irradiation of the long lived nuclear waste in accelerator driven systems (ADS) is expected to enable a reduction of the radiotoxic inventories sent to geologic repository by a factor of 100. In order to implement such systems, experimental and theoretical work on materials properties under neutron and proton irradiation is needed to assess the feasibility of technical options such as uranium free nitride fuels and liquid lead/bismuth spallation targets.

Position 1)

Modelling and optimisation of plutonium nitride fuel pins to be irradiated in the R2 reactor at Studsvik. Applicants should have documented experience in either neutronics simulations and/or complex geometry Monte Carlo simulations. FORTRAN fluency is required, as part of the work includes modification of Monte Carlo codes to be used in the project.

Duration: 24 months

Position 2)

Modelling of irradiation damage in Fe-Cr alloys subject to hard spectrum neutron and proton fields. Applicants should have documented experience in solid state molecular dynamics simulations and/or density functional treatment of transition metals. C fluency is required, as part of the work includes modification of molecular dynamics codes to be used in the project.

Duration: 12 months

The working environment at the department of Nuclear and Reactor Physics is very dynamic with plenty of opportunities for travel and lively discussion. The computer park consists of dedicated Linux clusters to be significantly upgraded for the projects in question. Salaries depend on experience, but are above Swedish academic average. As both projects will start on September 1st 2000, applicants are urged to send their CV:s together with a list of reference persons by E-mail to janne@neutron.kth.se as soon as possible.

Turn the tide and join the ride towards a sustainable Nuclear Energy!

Janne Wallenius, Nuclear & Reactor Physics, Lindstedtsvgen 24, KTH, 100 44 Stockholm, Sweden

Tel: 08 - 790 6395, Fax: 08 - 106 948, Mobile: 0709 - 527 591, WWW: <http://www.neutron.kth.se>

POSTDOCTORAL POSITION, AFRL HANSCOM ION CHEMISTRY LABORATORY

Our laboratory uses three unique fast flow tubes to measure ion-molecule kinetics of interest to the Air Force. The combination of instruments covers a temperature range of 90 - 1800 K, a pressure range of 0.2 to 700 Torr, and a kinetic energy range of 0.01 to 0.5 eV. The combination of temperature and kinetic energy measurements allows us to study reactivity as a function of rotational energy and vibrational state. A supersonic cluster source allows measurements of large clusters. A prominent area of interest involves using plasmas to enhance combustion in jet engines. This entails both making laboratory measurements of key ion reactions with fuel components and combustion byproducts and computer modeling of the combustion processes. Another combustion project involves ion nucleation of soot. Other interests include interactions of radio waves with vehicle generated plasmas around hypersonic vehicles and ion chemistry schemes for trace neutral detection.

Albert Viggiano, Skip Williams or Susan Arnold; Air Force Research Laboratory / VSBP, 29 Randolph Road, Hanscom AFB MA 01731-3010

781-377-4028 (Viggiano), 781-377-2076 (Williams), 781-377-1683 (Arnold),

albert.viggiano@hanscom.af.mil, skip.williams@hanscom.af.mil, susan.arnold@hanscom.af.mil

b. Preprints

Photodissociation of polarized diatomic molecules in the axial recoil limit: control of atomic polarization.

J. Chem. Phys.

JG Underwood & I Powis

School of Chemistry, University of Nottingham, Nottingham NG7 2RD UK

A quantum mechanical treatment of photofragment angular momentum polarization following photodissociation of a (possibly polarized) diatomic molecule is presented which includes AM coupling between the two fragments. The formalism treats coherent excitation of dissociative surfaces and the consequences of non-adiabatic coupling between surfaces. Possibilities for exploiting parent molecules polarization in order to control fragment polarization are discussed.

Crossed molecular beams investigation of elementary chemical reactions relevant to polycyclic aromatic hydrocarbons (PAHs) in outflow of carbon stars and hydrocarbon rich planetary atmospheres

Planetary and Space Science 48, 483-492 (2000)

R.I. Kaiser, O. Asvany, Y.T. Lee

Laboratory investigation the formation of unsaturated nitriles in Titans atmosphere

Planetary and Space Science 48, 447-462 (2000).

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

Crossed molecular beam experiments of radical-neutral reactions relevant to the formation of hydrogen deficient molecules in extraterrestrial environments

IAU Series

R.I. Kaiser, N. Balucani, O. Asvany, Y.T. Lee

The reaction of benzene with ground state carbon atoms, $C(^3P_j)$

J. Chem. Phys.

H.F. Bettinger, P.v.R. Schleyer, P.R. Schreiner, H.F. Schaefer III, R.I. Kaiser, Y.T. Lee

A combined crossed beam and ab initio investigation on the reaction of carbon species with C₄H₆ isomers I: the 1,3-butadiene molecule, H₂CCHCHCH₂ (X¹A)

J. Chem. Phys.

I. Hahndorf, H.Y. Lee, A. Mebel, S.H. Lin, Y.T. Lee, R.I. Kaiser

A combined crossed beam and ab initio investigation on the reaction of carbon species with C₄H₆ isomers II: the dimethylacetylene molecule, H₃CCCCH₃ (X¹A₁)

J. Chem. Phys.

L.C.L. Huang, H.Y. Lee, A. Mebel, S.H. Lin, Y.T. Lee, R.I. Kaiser

Crossed beam reaction of cyano radicals with hydrocarbon molecules III: Chemical dynamics of vinylcyanide (C₂H₃CN; X¹A) formation from reaction of CN(X²Σ_g⁺) with ethylene, C₂H₄(X¹A_g)

J. Chem. Phys.

N. Balucani, O. Asvany, A.H.H. Chang, S.H. Lin, Y.T. Lee, R.I. Kaiser, Y. Osamura

Crossed beam reaction of cyano radicals with hydrocarbon molecules IV: Chemical dynamics of cyanoacetylene (HCCCN; X¹Σ⁺) formation from reaction of CN(X²Σ⁺) with acetylene, C₂H₂(X¹Σ_g⁺)

J. Chem. Phys.

L.C.L. Huang, A.H.H. Chang, O. Asvany, N. Balucani, S.H. Lin, Y.T. Lee, R.I. Kaiser, Y. Osamura

Neutral-neutral reactions in the interstellar medium III: Formation of Nitriles via reaction of cyano radicals, CN(X²Σ⁺), with unsaturated hydrocarbons

ApJ. (submitted March 2000).

N. Balucani, O. Asvany, L.C.L. Huang, Y. T. Lee, R.I. Kaiser, Y. Osamura, H.F. Bettinger, P.v.R. Schleyer, H.F. Schaefer III

Observation of borirene from reactions of boron atoms with ethylene

J. Am. Chem. Soc. (submitted April 2000).

N. Balucani, O. Asvany, Y. T. Lee, R. I. Kaiser, N. Galland, Y. Hannachi

Neutral-neutral reactions in the interstellar medium IV: the formation of C₅H₅ isomers as potential key intermediates to PAH like molecules

ApJ (submitted May 2000).

R.I. Kaiser, H.Y. Lee, A.M. Mebel, Y. T. Lee

Nucleation of hydrogen deficient carbon clusters in circumstellar envelopes of carbon stars

World Scientific Press (submitted June 2000).

C.C. Chiong, O. Asvany, N. Balucani, Y.T. Lee, R.I. Kaiser

Neutral- neutral reactions in the interstellar medium V: Elementary reactions of C₆H₅ and C₆H₆

ApJ (submitted July 2000).

R.I. Kaiser, O. Asvany, I. Hahndorf, Y. T. Lee, L. Vereecken, J. Peeters, H.F. Bettinger, P.v. R. Schleyer, H.F. Schaefer

Inversionless Gain in an Optically-Dense Resonant Doppler-Broadened Medium

Optics Express (<http://www.opticsexpress.org/oearchive/source/22947.htm>)

A. K. Popov, S. A. Myslivets and T. 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

Resonant nonlinear-optical interference processes in four-level Doppler-broadened media are studied, where specific features of amplification and optical switching of short-wavelength radiation in a strongly-absorbing resonant gas under coherent quantum control with two longer wavelength radiations are investigated. Calculations are carried out for sodium dimer vapor.

Four-Wave Mixing at Maximum Coherence and Eliminated Doppler Broadening Controlled with the Driving Fields

European Physics Journal D - EPJdirect (<http://link.springer.de/link/service/journals/10105/tocs/t0002d.htm>)

A. K. Popov, Alexander S. Bayev, Thomas F. George* and Vladimir M. Shalaev Office of the Chancellor / Department of Chemistry and Physics & Astronomy University of Wisconsin-Stevens Point Stevens Point, WI 54481-3897

tgeorge@uwsp.edu

New feasibility of coherent quantum control of four-wave mixing processes in a resonant Doppler-broadened medium is studied, where we propose a technique which enables one to enhance the quantum efficiency of nonlinear optical conversion.

Representation of potential energy surfaces by discrete polynomials: proton transfer in malonaldehyde.

Physical Chemistry Chemical Physics

V. Aquilanti, G. Capecchi and S. Cavalli

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

C. Adamo and V. Barone

Dipartimento di Chimica, Università Federico II, I-80134 Napoli, Italy

A new method for the expansion of potential energy surfaces has been developed exploiting the peculiar properties of Hahn polynomials, a class of orthogonal polynomials of a discrete variable which generalize 3j vector coupling coefficients of angular momentum algebra.

Angular momentum coupling schemes for molecular collisions: the stereodirected representation

Physics Essays, Special Issue in Honor of Ugo Fano

Vincenzo Aquilanti, Simonetta Cavalli and Alessandro Volpi

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

The tools of angular momentum algebra, and in particular the limiting relationships known as semiclassical limits provide alternative representations for the quantum mechanical scattering matrix and the description of steric effects in molecular collisions. Implications for reactive scattering theory, an explicit discretization algorithm (hyperquantization) and numerical results are also outlined.

Ab Initio Dynamics of $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ Reaction: a New Potential Energy Surface and Quantum Mechanical Cross Sections

Mol. Phys.

P. Palmieri(a), C. Puzzarini(a), V. Aquilanti(b), G. Capecchi(b), S. Cavalli(b), D. De Fazio(b), A. Aguilar(c), X. Gimenez(c), J.M. Lucas(c)

(a) Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, 40126 Bologna, Italy

(b) Dipartimento di Chimica, Università di Perugia, 06123 Perugia, Italy

(c) Department de Química Física, Universitat de Barcelona, 08028 Barcelona, Spain

More than 1400 ab-initio points at MRCI level and a many-body expansion with a large number of terms permits an accurate analytical representation of the potential energy surface with a root-mean-square deviation < 12 meV. A new hyperquantization algorithm has been implemented to obtain quantum mechanical integral cross sections which are compared with previous calculations and with experimental results.

c. Conferences

1. 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

BRIJUNI CONFERENCE APPLICATION FORM

NAME (including accompanying person/s)

.....
.....

ADDRESS (including email)

.....
.....
.....

TITLE OF CONTRIBUTION

.....
.....

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

LOCAL ORGANIZING COMMITTEE

VLADIMIR SPIRKO, chairman

STEPAN 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: praha2k@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.

ELECTRONIC ABSTRACT SUBMISSION (EAS)

We offer fully automated electronic abstract submission. We employ slightly modified versions of the programs written by Dr. Sergey Panov and Prof. Terry A. Miller for the Ohio State University Symposia on Molecular Spectroscopy. We are very grateful to Dr. Panov and Prof. Miller for making these programs available to us.

To submit your abstract electronically, you must download the instructions. To accomplish this, do one of the following:

- * Access the PRAHA2000 WWW site at <http://www.chem.uni-wuppertal.de/conference/> and follow the menu to electronic abstract submission instructions, or
- * Access our anonymous ftp server at praha.jh-inst.cas.cz (or ftp.uni-wuppertal.de) and download the file submit, or
- * Send an email to eas@praha.jh-inst.cas.cz The email should contain only the subject line: EAS

Instructions.

When you have completed your electronic abstract, just email it to our test address for viewing or to the above email address for actual submission. Upon receipt, your document will be processed by a LaTeX-2e compiler and you will automatically receive an email reply indicating either a successful submission or a problem. If you submit electronically and you receive confirmation of a successful submission, you need do nothing more. Once you have successfully submitted your abstract, DO NOT resubmit it or a "revised" copy electronically. DO NOT send us an additional paper copy. Either action could result in your abstract being included twice in the program. Please note that we can only handle one format for electronic submission. LaTeX was chosen because of its support by several American professional societies and widespread use in the worldwide scientific community.

SUBMISSION OF ABSTRACTS BY PAPER MAIL

You are strongly discouraged from submitting abstracts by paper mail. Please use the electronic abstract submission facility if at all possible. However if you must, then submit two printed copies of each abstract to PRAHA2000, c/o Dr. Stepan Urban, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejskova 3, CZ-18223 Praha 8, Czech Republic, before May 1st 2000.

You can give your contribution as a poster (default) or as a talk. If you prefer a talk, please write the word "TALK" in the lower left-hand corner of the page (i.e., outside the area that will be reproduced photographically) together with the number of minutes required (max. 15').

A correct reproduction of your abstract requires that the rules in this paragraph be followed:

- * Each abstract should be typed on a single sheet of A4 (210 x 297 mm) or letter size (8.5 x 11") paper.
- * The typed area should not exceed 150 x 237 mm as indicated on the model abstracts. Anything outside this area will be cut off.
- * The typed area should be centered on the page so that the margins are at least 30 mm wide.
- * The quality of the typing should be sufficient for photographic reproduction.
- * Each abstract should be headed by the title of the communication together with the names, affiliations, and mailing addresses of the authors.
- * Names of authors who will be present at the conference should be underlined.

We would like the abstracts in the conference book to be of uniform appearance. Hence we would much appreciate it if you would use 12 pts Roman or Times New Roman font with a line spacing of 1.5, set the abstract title in bold capitals, the authors' names in small capitals, and the affiliations and addresses in italics. Owing to the limited time available for contributed talks, we shall probably not be able to grant all applications for oral presentations, and we may find it necessary to shorten some contributed talks. If we

must shorten your talk, or turn it into a poster, we will inform you about this as soon as possible.

PRAHA2000 Prizes

At the meeting, PRAHA2000 Prizes will be awarded for the best student contributions.

The prize will consist of a diploma and the recipients will be given a selection of books.

In order to be eligible for a PRAHA2000 Prize, a student must

- * be primary (first) author of the work being presented;
- * for talks: be the actual presenter of the talk;
- * for posters: assume the sole responsibility for the presentation during the entire session, and
- * be working for a Ph.D. or having completed it within the last 12 months (at the time of the meeting).

If a student wishes to compete for the PRAHA2000 Prize, he or she should indicate this in the comment area of the abstract (due by May 1st, 2000) for the talk or poster to be judged, if this abstract is submitted electronically. The research supervisor should then send a letter (to PRAHA2000, c/o Dr. Stepan Urban, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejskova 3, CZ-18223 Praha 8, Czech Republic) certifying that the student meets all of the above requirements. The letter of certification should mention the unique identification (in the form "pnnn", where "nnn" is a three-digit number) assigned to the abstract by the electronic abstract submission software. The letter of certification is not a nomination letter and will not be considered by the prize judges. If the abstract is submitted by paper mail, the letter of certification should accompany it.

Accommodation

Reservation of accommodation should be made before May 1st 2000 (See the registration form). Single and double rooms are available in student dormitories within easy walking distance of the conference site. For participants who prefer to stay in hotels, we will attempt to provide comfortable rooms. However, the hotels may be located some distance from the conference site. In hotels of category ***, the rooms have telephones, TV sets, private bathrooms and toilets. Meals will be available at the student cafeteria for euro 12 per day.

Registration

You should register before May 1st 2000

(See the registration form). If you have submitted a preregistration form, you should receive the registration form by paper mail during March 2000. Otherwise, you can request a registration form in one of the following ways:

- * Download the PostScript file reg.ps or the WORD97 document reg.doc from our ftp server. These files are formatted for A4 paper. If you use letter size (8.5 x 11 inch) paper, please download reg_lett.ps or reg_lett.doc. The files contain PostScript and WORD97 versions of the registration form. You can print out the files and fill out the printed form, or fill out the WORD document electronically and
- * Contact the local organizers (by paper mail, phone, fax, or e-mail. and give them your paper mail address.
- * You can also request a blank registration form from our WWW fill-out form.

Registration fee

The registration fee is

Before June 1st, 2000

Students: euro 110

Other participants: euro 180

Accompanying persons: euro 120

After June 1st, 2000

Students: euro 130

Other participants: euro 200

Accompanying persons: euro 140

On site payment, 2000

Students: euro 135

Other Participants: euro 205

Accompanying persons: euro 145

If you claim the reduced fee for students, please submit a copy of your student identity card or its equivalent.

You can pay by bank cheque (drawn on Ceskoslovenska obchodni banka if possible), money order, Eurocheque, Eurocard/Mastercard, VISA, and by bank transfer to Recipient: Ustav Fyzikalni Chemie, Dolejskova 3, 182 23 Praha 8.

Account Number: 01-09507280/0300

Bank: Ceskoslovenska obchodni banka, Na prikope 14, 115 20 Praha, Czech Republic.

SWIFT: CEKOCZPPRA

Purpose of Payment: Conference Fee / ;participant name;

Cheques should be made payable to Ustav Fyzikalni Chemie. Please do not send postal cheques or personal cheques.

In case the payment covers the costs of more than one participant, please send us (for example by e-mail to praha2k@jh-inst.cas.cz) a complete list of their names. Do not forget to mention the name of the participant given under "Purpose of Payment" above.

You can cancel your registration until August 1st, 2000. Your payment will be refunded with a euro 20 deduction for administrative purposes.

Social program

During the conference there will be a reception, a concert followed by a light snack, a sight-seeing trip, and excursions for accompanying persons.

3rd circular with meeting information

June 2000. This circular will give instructions for preparing posters.

WWW server

The conference has a home page on the World Wide Web providing up-to-date information. Start browsing at URL

<http://www.chem.uni-wuppertal.de/conference/>

ftp server

The conference has ftp servers at

[ftp.uni-wuppertal.de](ftp://ftp.uni-wuppertal.de)

and

[praha.jh-inst.cas.cz](ftp://praha.jh-inst.cas.cz)

Use "ftp" or "anonymous" as user id and enter your complete e-mail address as password. The conference files are in the directory pub/praha2k and most of them are mirrored at the two locations. The ASCII file read.me gives a list of the files available at Wuppertal and describes their contents.

Preliminary program

Sunday:

09:00 Opening Lectures, 10:30 Posters, 12:00 Lunch, 14:00 Lectures, 16:00 Posters, 18:00 Reception

Monday:

09:00 Lectures, 10:30 Posters, 12:00 Lunch, 14:00 Lectures, 16:00 Posters, 18:00 Dinner

Tuesday:

09:00 Lectures, 10:30 Posters, 12:00 Lunch, 14:00 Free Afternoon, 18:00 Dinner

Wednesday:

09:00 Lectures, 10:30 Posters, 12:00 Lunch, 14:00 Lectures, 18:00 Concert, Snack

Thursday:

09:00 Lectures, 10:30 Lectures, 12:00 Lunch

3. 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>

4. 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

5. 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

6. 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>

7. 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.

8. 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)

9. 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)

10. 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

11. 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.

12. 2001 GORDON CONFERENCE ON MOLECULAR ENERGY TRANSFER

January 14-19, 2001, Sheraton Harbortown Resort Ventura, California

Co-chairs: Joel M. Bowman (Emory University)

Hanna Reisler (University of Southern California)

Updated information can be found at <http://www.grc.uri.edu/programs/2001/met.htm>

13. 6th Winter Gordon Research Conference on GASEOUS IONS: STRUCTURES, ENERGETICS, AND REACTIONS

February 25 - March 2, 2001, Ventura Beach Hotel, Ventura California

Peter B. Armentrout, Chair, Department of Chemistry, University of Utah, 315 S. 1400 E. Rm 2020, Salt Lake City, UT 84112, USA

armentrout@chemistry.utah.edu, 801 581 7885, FAX: 801 581-8433

Terry B. McMahon, Vice Chair, Department of Chemistry, University of Waterloo, Waterloo, ON N2L 3G1, Canada

mcmahon@uwaterloo.ca, 519 888-4591, FAX: 519 746-0435

For complete information, visit <http://www.grc.uri.edu/programs/2001/gaseous.htm> or <http://www.chem.utah.edu/ion-grc/>.

The 2001 Gordon Conference on Gaseous Ions: Structures, Energetics, and Reactions is the 6th in the series of biennial conference established to provide a forum for scientific exchange among individuals interested in the spectroscopy and structures of ions, the thermochemistry of ionic processes, and the mechanisms and dynamics of gaseous ion reactions. The program for the 2001 conference will draw from a selection of areas of intense current interest, and includes sessions on Analytical Mass Spectrometry, Clusters, Environment and Aerosols, Ion Spectroscopy, Ions in Nanodroplets, Noncovalent Ion Interactions, Organic Ions, and Organometallic Ion Chemistry.

The conference will begin on Sunday evening with both an oral and a poster session. Poster sessions will continue on Monday, Tuesday, and Wednesday evenings. The Conference will climax on Thursday evening with a banquet, an after dinner speaker, and an after dinner dance. Departure is on Friday morning.

Application forms for the Gordon Conference must be submitted to the GRC office, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892-0984. Tel. 401 783-4011 (-7644 fax). Online applications are encouraged at www.grc.uri.edu. Applications are encouraged by January 14, 2001. Deadline for registration at reduced rate is 4 weeks prior to the conference, i.e. January 28, 2001.

Program at a Glance

Sunday Evening Ions in Nanodroplets: Evan Williams/ Gereon Niedner-Schatteberg/ Jack Beauchamp

Monday Morning Organometallic Ion Chemistry: Karl Irikura/ Doreen Leopold/ Atsushi Nakajima/ Jim Weisshaar

Monday Evening Environment and Aerosols: Al Viggiano/ Dave Feller/ Tom Baer

Tuesday Morning Analytical Mass Spectrometry: Veronica Bierbaum/ Alan Marshall/ Julie Leary/ Michael Gross

Tuesday Evening Clusters: Will Castleman/ Kent Ervin/ Lai-Sheng Wang

Wednesday Morning Organic Ions: Tom Morton/ Frank Turecek/ Richard O'Hair/ Einar Uggerud

Wednesday Evening Noncovalent Ion Interactions: Christoph Schalley/ Gilles Ohanessian/ Mary Rodgers

Thursday Morning Ion Spectroscopy: Mike Duncan/ Benoit Simard/ Mattanjah de Vries/ Bernd. Brutschy

Thursday Evening Helmut Schwarz

14. 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

15. 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

16. XVIIIth Conference on the Dynamics of Molecular Collisions

July 15-20, 2001 Copper Mountain Resort and Conference Center Copper Mountain, Colorado

James T. Muckerman, Chair Department of Chemistry Brookhaven National Laboratory Upton, NY 11973-5000 USA

Laurie J. Butler, Vice-Chair Department of Chemistry University of Chicago Chicago, IL 60607 USA

Description of the Conference

The Dynamics of Molecular Collisions Conference focuses on all aspects of molecular collisions—experimental and theoretical studies of elastic, inelastic, and reactive encounters involving atoms, molecules, ions, clusters, and surfaces—as well as half collisions—photodissociation, photo-induced reaction, and photodesorption. The Conference began as a Gordon Conference in 1965, and though it now operates independently, retains the Gordon Conference format and spirit.

Meeting Site

The meeting will be held at Copper Mountain Resort and Conference Center located 75 miles due west of Denver, Colorado on Interstate 70. Nestled in the heart of the Rocky Mountains, Copper Mountain Resort offers abundant recreational facilities, including 18 holes of championship golf. Conference attendees will receive complimentary access to the Copper Indoor Racquet and Athletic Club, which features cardio equipment, weight room, indoor pool and jacuzzi. There are over 47 miles of paved bike paths, acres of mountain biking, tennis, and swimming. Copper offers everything you would expect to find in the mountains - horseback riding, hiking, white water rafting, fishing and a scenic narrow gauge railroad.

More information on Copper Mountain is available at the Resort web site, <http://www.ski-copper.com>.

Meeting Program

The XVIIIth Conference will have morning sessions on Monday through Friday, and evening sessions Monday through Thursday. In each session the first talk will be an overview of the topic of that session. Afternoons are free for discussions and recreation. Session topics and speakers will be announced in the early fall of 2000.

A poster session will follow the formal session on Monday through Thursday evenings. Attendees are strongly encouraged to present posters. "Camera ready" poster abstracts for inclusion in the conference program book should be submitted to the conference chair by June 1, 2001. These submissions may be in either hard copy or electronic (PC Word or WordPerfect) form. Faxes or email (except "attachments") are NOT acceptable.

Lodging and Meals

Reservations for accommodations must be made directly to Copper Mountain Resort. (Registration for the DMC Conference is a separate process [see below].) When making your reservations at Copper Mountain Resort, you must identify yourself as an attendee of the Dynamics of Molecular Collisions Conference to obtain the discounted rate. The cost of five nights of lodging (Sunday through Thursday) and five days of meals (dinner Sunday through lunch Friday), based on double occupancy is, \$605. A block of hotel-style double rooms has been reserved for DMC Conference attendees. Single rooms, subject to availability, may also be reserved at a discounted (but higher) rate. You can reach Copper Mountain by phone at 1-800-458-8386. CMR hopes to offer web registration to attendees of the DMC Conference by the spring of 2001.

Registration

Registration forms for the DMC Conference will be available for downloading and/or printing from a PDF document on the DMC Conference web page at http://www.gpmd.bnl.gov/dmc_conf/

They will also be mailed upon request. Completed registration forms should be sent to "DMC Conference, c/o James T. Muckerman, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000." Be sure to enclose the appropriate payment. The fee for early registration (received on or before April 16, 2001) is \$100. The registration fee after April 16 is \$150.

Bus Transportation

Resort Express offers regular and frequent limosine service to Copper Mountain from the Denver International airport. The one-way travel time is 90 minutes. In 1999, the discounted group round trip fare was \$74 per person. If there is sufficient interest expressed to the conference chair, buses from the Denver International airport (each with a capacity of 47 persons) can be arranged for a somewhat lower round-trip fare.

Graduate Student Scholarships

Graduate student scholarship awards will be announced at the Conference. The number and amount of these scholarships will depend on available funds.

Watch the DMC web page for updated information.

Conference Contacts

Email: muckerma@bnl.gov Fax: 631-344-5815 Voice: 631-344-4368 Mail: J.T. Muckerman Chemistry Department Brookhaven National Laboratory Upton, NY 11973-5000

17. 26th International Symposium on Free Radicals.

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

Chairman: Piergiorgio Casavecchia (Universit di Perugia). 26th INTERNATIONAL SYMPOSIUM ON FREE RADICALS

<http://www.chm.unipg.it/chimgen/mb/cong/FreeRadicals2001.html> e-mail: freeradicals@mail.dyn.unipg.it

The 26th International Symposium on Free Radicals will be held at "La Cittadella" in Assisi, ITALY, 2-7 September 2001. Assisi is a unique medieval town rich of art masterpieces. It is located in a beautiful landscape, 25 km east of Perugia, the capital of the Umbria region known as the "green heart" of Italy. The

Symposium will address the physical and chemical properties of FREE RADICALS, including paramagnetic molecules, ions, molecules in excited states and short-lived species.

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

The local organizing committee includes the members of the Perugia Molecular Beam Group (home page: <http://www.chm.unipg.it/chmgen/mb/mb.html>) of the Department of Chemistry (home page:

<http://www.chm.unipg.it>) of the University of Perugia (home page: <http://www.unipg.it>): V. Aquilanti, N. Balucani, B. Brunetti, R. Candori, D. Cappelletti, S. Cavalli, S. Crocchianti, S. Falcinelli, G. Grossi, A. Lagan, G. Liuti, E. Luzzatti, F. Pirani, F. Vecchiocattivi, G.G. Volpi.

The purpose of the 2001 Symposium is to survey recent advances, undertake stimulating discussions, generate new ideas, and map out future directions in the field of free radical chemistry. The scientific program will cover a wide variety of topics by papers and discussions:

* Spectroscopy of radicals * Structure of free radicals * Reaction Dynamics and Kinetics of free radicals, experiment and theory * Inelastic collisions of free radicals * Photodissociation of free radicals * Femto-second dynamics * Free radicals and atmospheric-chemistry * Free radicals and astro-chemistry * Free radicals and combustion-chemistry * Free radicals as reaction intermediates * Molecular ions and molecules in excited states * Free radicals in applied research * Production and observation techniques

There will be several invited talks covering the listed topics above. Contributed papers will be presented in poster sessions with a brief introduction by the author. A few contributions will be selected for oral presentation as Hot Topics.

Information will be continuously updated on the Symposium web-site and on March 2001 e-mailed to those on the Conference mailing list. To be added to the mailing list, please fill out the following form and mailed or fax it. You can also pre-register at our Web Site :

<http://www.chm.unipg.it/chimngen/mb/cong/FreeRadicals2001.html>

***** PRE-REGISTRATION FORM *****

26th INTERNATIONAL SYMPOSIUM ON FREE RADICALS September 2-7, 2001 "La Cittadella",
Assisi, ITALY

To receive further information, please fill the registration form available at the Symposium web site <http://www.chm.unipg.it/chimngen/mb/cong/FreeRadicals2001.html> and return it (by FAX: +39 075 585 5606, or e-mail: freeradicals@mail.dyn.unipg.it) before February 28, 2001.

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).