

# Molecular Dynamics News

number 97, October 1998

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

The format for MDN is

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 has been accepted - otherwise state *unpublished*).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

MDN is edited by Prof. Vincenzo Aquilanti, Dipartimento di Chimica dell' Università, 06123 Perugia, Italy (electronic mail: AQUILA@DYN.UNIPG.IT) and Prof. Roger W. Anderson, Dept. of Chemistry, University of California, Santa Cruz, CA 95064, U.S.A. (electronic mail: ANDERSO@CATS.UCSC.EDU).

Send all material for issue 98 to Prof. R. Anderson (You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#97). The closing date for issue number 98 is December 1, 1998.

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

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

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

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# ANNOUNCING ELECTRONIC DELIVERY OF MDN

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

## 1. Electronic mail to subscribers

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

## 2. World Wide Web

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

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

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

### **The MDN e-mail list continues, as detailed below**

#### MOLECULAR DYNAMICS NEWS EMAIL LIST

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

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

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

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

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

If you would like a list of the current members, send a message containing the line  
review molecular-dynamics-news

to the address [mailbase@mailbase.ac.uk](mailto: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.**

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

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join spectroscopy-group John Kennedy
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## **a. Open Positions**

### **FACULTY**

#### **FACULTY POSITION IN LASER PHYSICS, DEPARTMENT OF PHYSICS, UNIVERSITY OF WATERLOO**

The Department of Physics, University of Waterloo, invites applicants for a tenure-track position at the Assistant Professor level in the field of experimental laser physics, with applications in one or more of the following areas: ultrafast phenomena, materials processing, biomaterials, particle trapping and manipulation, to begin in September 1999. Candidates in all areas of laser physics will be considered. In exceptional cases appointment at a more senior level will be considered. Further information about the Department can be found on our WEB page <http://www.science.uwaterloo.ca/physics>.

Applicants must have a Ph.D. degree, a record of research accomplishments normally achieved through postdoctoral experience, and promise for excellence in teaching. Salary range commensurate with qualifications and experience. Candidates should submit by regular mail a curriculum vitae, an outline of research accomplishments, a brief research plan, and a statement of their teaching goals. Arrangements should be made for three letters of reference to be sent. Materials should be received by November 2, 1998 and addressed to Dr. D. Strickland, Laser Physics Search Committee, Department of Physics, University of Waterloo, Waterloo, Ontario, CANADA, N2L 3G1, TEL: (519) 888-4567, Ext. 6831; E-mail: [PHYSICS@UWATERLOO.CA](mailto:PHYSICS@UWATERLOO.CA).

In accordance with Canadian immigration requirements, this advertisement is directed to Canadian citizens and permanent residents. The University of Waterloo encourages applications from all qualified individuals, including women, members of visible minorities, native peoples, and persons with disabilities. This appointment is subject to the availability of funds.

#### **FACULTY POSITION IN EXPERIMENTAL PHYSICS The University of Chicago**

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

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

#### **PHYSICAL/BIOPHYSICAL CHEMISTRY FACULTY POSITION**

We are pleased to announce that a faculty position in physical/biophysical chemistry is available at the University of Puerto Rico at Rio Piedras. The following ad appeared in Science in May 1998.

The Department of Chemistry of the University of Puerto Rico-Rio Piedras invites applications for a tenure-track position at the Assistant Professor level beginning as early as August 1998. The successful candidate will be expected to develop an active and competitive research program in Ultrafast (fs and/or ps) Spectroscopy applied to biomolecular processes and biomedical problems. Possible areas could include Electron Transfer, Protein Dynamics, and Fast Processes in Photobiology. A generous start-up package, funded by the National Institute of Health through the Research Centers at Minority Institutions Programs, will be made available to the successful candidate. Applicants should have a demonstrated record of

scholarship, research experience and a strong interest in fast processes in biochemical systems. In addition, the successful candidate should have a strong interest developing and teaching classes at both the undergraduate and graduate levels. A Ph.D. in chemistry, biochemistry, biophysics or related fields is required. Please submit a complete Curriculum Vitae and publication record, a brief summary (3-5 pages) of research plans and three letters of reference by June 1, 1998 to Reginal Morales, Chair, Department of Chemistry, University of Puerto Rico, P.O. Box 23346, University Station, San Juan, Puerto Rico 00931 (e-mail: rmorale@upracd.upr.clu.edu).

### **FACULTY POSITION IN EXTRAGALACTIC ASTRONOMY/COSMOLOGY, DEPARTMENT OF PHYSICS, UNIVERSITY OF WATERLOO**

The Department of Physics, University of Waterloo, invites applicants for a tenure-track position at the Assistant Professor level in the area of extragalactic astronomy to begin in September 1999. We are particularly interested in a person who has aptitude with data in the areas of background radiation, large-scale structure of the Universe, or galaxy formation. Outstanding candidates in other areas of astrophysics and gravitation will also be considered. In exceptional cases appointment at a more senior level will be considered. Further information about the Department can be found on our Web page at <http://www.science.uwaterloo.ca/physics>.

Applicants must have a Ph.D. degree, a record of research accomplishments normally achieved through postdoctoral experience, and promise for excellence in teaching. The salary range will be commensurate with qualifications and experience. Candidates should submit by regular mail a curriculum vitae, an outline of research accomplishments, a brief research plan, and a statement of their teaching goals. Arrangements should be made for three letters of reference to be sent. Materials should be received by November 2, 1998 and addressed to Dr. R.B. Mann, Astrophysics Hiring Committee, Department of Physics, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1. TEL: (519) 888-4567, Ext. 6831; e-mail: [physics@uwaterloo.ca](mailto:physics@uwaterloo.ca). In accordance with Canadian immigration requirements, this advertisement is directed to Canadian citizens and permanent residents. The University of Waterloo encourages applications from all qualified individuals, including women, members of visible minorities, native peoples, and persons with disabilities. This appointment is subject to the availability of funds.

### **LECTURESHIP University of Durham**

A lectureship is available in the Department of Chemistry at the University of Durham (Research rating: 5; Teaching assessment rating; excellent). The position is for an initial period of 3 years, extendable for a further 2 years, and with some potential for continuation to a permanent position.

Applicants should have a Ph D in chemistry or physics and research interests in experimental or theoretical physical chemistry or chemical physics. The successful candidate will be required to teach undergraduates in general aspects of physical and theoretical chemistry (including mathematics for chemists) and develop a successful research programme.

Further information about the Department and the University are available via the Department's Web page at <http://www.dur.ac.uk/~dch0www/>

Informal enquiries may be made to Prof. Robin K. Harris (tel. 0191 374 3121) or email [R.K.Harris@durham.ac.uk](mailto:R.K.Harris@durham.ac.uk)

Further details and an application form may be obtained from the Director of Personnel, University of Durham, Old Shire Hall, Durham, DH1 3HP (tel. 0191 374 7258; FAX 0191 374 7253; email [Acad.Recrut@durham.ac.uk](mailto:Acad.Recrut@durham.ac.uk)). The closing date for applications is 16 July 1998. Enquiries should quote reference no. A804D.

### **Department of Chemistry, YORK UNIVERSITY**

Tenure-track Position in Experimental Physical Chemistry of Materials

Applications are invited for a tenure-track faculty position in experimental physical chemistry, subject to

budgetary approval. Candidates should be physical chemists with research interests in some aspect of materials science and have a strong record of accomplishment in a related research area. The successful candidate will be expected to direct an active research programme, and to develop and teach courses at the graduate and undergraduate levels. Qualified candidates will be considered at the Assistant Professor or higher level commensurate with experience. Candidates should provide a curriculum vitae, a statement of research interests and plans for a proposed programme of research, and should arrange for three letters of reference to be sent to: Dr. J.M. Goodings, Chair, Materials Search Committee, York University, 4700 Keele Street, Toronto (North York), Ontario M3J 1P3, Canada. Review of applications will begin November 1, 1998. York University is implementing a policy of employment equity including Affirmative Action for women faculty. Qualified men and women are invited to apply. In accordance with Canadian immigration requirements, this advertisement is directed toward Canadian citizens and permanent residents. Dr. Chester Sadowski, Chair (chesters@turing.sci.yorku.ca) Department of Chemistry Faculty of Pure and Applied Science York University, North York, Ontario, M3J 1P3, Canada Telephone: (416)736-2100 (ext.77714) or (416)736-5246 FAX: (416)736-5936

## POST DOCTORAL AND VISITING

### POSTDOCTORAL POSITION AVAILABLE

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

For more information about recent and ongoing research projects see

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

For any other information please contact me at [tamar@mahler.sims.nrc.ca](mailto:tamar@mahler.sims.nrc.ca) or at Tel. 613-990-0945.

– e-mail: [tamar.seideman@nrc.ca](mailto:tamar.seideman@nrc.ca) <http://gold.nrc.ca/~tamar> [tamar@mahler.sims.nrc.ca](mailto:tamar@mahler.sims.nrc.ca)

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

### POSTDOCTORAL POSITION, New York University

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

New York city provides a unique and exciting environment for any person who is interested in big city living.

John Z.H. Zhang Professor of Chemistry Department of Chemistry New York University New York, NY 10003 Tel. 212-998-8412 Fax. 212-260-7905 [zhang@risc.nyu.edu](mailto:zhang@risc.nyu.edu) [zhang@p150.chem.nyu.edu](mailto:zhang@p150.chem.nyu.edu)

<http://risc.nyu.edu>

### POSTDOCTORAL ASSOCIATE, Ohio State University

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

Information on our interests and several reprints and preprints are available at

<http://www.chemistry.ohio-state.edu/~mcbane/research.html>

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

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

#### **POSTDOCTORAL APPOINTMENT SEPTEMBER 1998**

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

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

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

#### **POSTDOCTORAL POSITIONS, Korea Advanced Institute of Science and Technology**

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

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

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

ROC.Tel:886-2-23645370;Fax:886-2-23620200; email:kaiser@po.iams.sinica.edu.tw.  
<http://po.iams.sinica.edu.tw/~kaiser>.

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

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

**POSTDOCTORAL POSITIONS, SRI International**

Postdoctoral Fellow positions are available in the Laser-Based Diagnostics Group of the Molecular Physics Laboratory at SRI International in Menlo Park, California. This group has extensive experience in the development of quantitative laser-based measurements in reactive gas phase environments which include flames, plasmas, and the atmosphere. Research activities include quantitative measurements in laboratory flames related to  $\text{NO}_x$  pollutants; development of spectroscopic strategies for detection of radicals such as  $\text{HO}_2$  and  $\text{HCO}$ ; collisional relaxation measurements to support quantitative laser-based measurement of radical species; and quantitative measurements of radical intermediate species to test the predictions of detailed models of flames and plasmas. The group includes David Crosley, Jay Jeffries, Gregory Smith, Leah Williams, and Jorge Luque. Menlo Park is located on the peninsula side of the San Francisco Bay between San Francisco and San Jose. One postdoctoral position is available immediately to replace a postdoctoral fellow departing for a permanent industrial job and a second postdoctoral position is anticipated. Experience with laser-based detection, chemical kinetics, collision dynamics, and spectroscopy of diatomic and triatomic radicals is desired. Salary for beginning postdoctoral fellows is approximately \$31,500, and increases with prior postdoctoral experience. Interested candidates should send a resume to Jay Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave. Menlo Park, CA 94025 or [Jeffries@mplvax.sri.com](mailto:Jeffries@mplvax.sri.com).

**POSTDOCTORAL POSITION, Colorado State University**

A postdoctoral position is available to study radical-surface interactions using a unique REMPI/TOFMS apparatus and to study metal-ligand charge transfer reactions using steady-state and time-resolved spectroscopy. The initial focus of the position will be to develop a ns pulsed Nd:YAG laser system for REMPI and transient absorption experiments. The position may eventually specialize in one of these areas. Experience with lasers, preferably ns pulsed and dye laser systems, is required. Additional desirable qualities include inorganic synthesis, knowledge of vacuum systems, and an ability and desire to work with graduate and undergraduate students. Further information on specific projects available may be found at <http://www.chm.colostate.edu/erf> and <http://www.chm.colostate.edu/cme>. Interested individuals should submit a curriculum vitae and names of three references to Prof. Ellen R. Fisher or Prof. C. Michael Elliott, Department of Chemistry, Colorado State University, Fort Collins, CO 80523-1872. Colorado State University is an EEO/AA Employer and strongly encourages applications from women and minorities. Ellen R. Fisher, Department of Chemistry, Assistant Professor of Chemistry, Colorado State University, Fort Collins, CO 80523-1872, (970)-491-5250 (office), (970)-491-1801 (FAX)

### **POSTDOCTORAL POSITION, University of Southern California**

A postdoctoral position is available to work on unimolecular and bimolecular reactions of molecules and radicals using product ion imaging and TOF/REMPI techniques. A short description is given below, and further information about our research can be found in my group's homepage:

<http://www-rcf.usc.edu/~reisler>.

Two machines are currently available, one devoted to crossed beams studies of bimolecular reactions and the other optimized for the production and detection of free radicals. The postdoc will be responsible for implementing recent improvements in resolution and data acquisition techniques, as well as for the application of the technique to processes important in combustion and in atmospheric chemistry. The ion imaging technique complements several others in our lab, e.g., LIF, IR/UV pumping with high-resolution OPO's, etc.

1. Unimolecular reactions of free radicals (e.g. hydroxymethyl, allyl) are studied using photofragment ion imaging with REMPI detection. Pyrolytic and photolytic production of radicals are implemented. Reactions proceeding via multiple pathways and involving nonadiabatic transitions and isomerization are emphasized, as well as state-specific effects enhanced by using multiple photon and double resonance pumping schemes.
2. Bimolecular Reactions of atoms and radicals are studied using imaging in a crossed molecular beam machine previously used in studies of state-selected collision induced dissociation. The postdoc will study reactions of atoms and radicals important in combustion and atmospheric processes, acquiring state-to-state dynamical information that is important in modeling.

Other related experiments carried out in my lab include:

3. Reactions of atomic carbon in pulsed molecular beams, in which both free and seeded ablation techniques are used to study insertion, abstraction and addition reactions of carbon.
4. Photoinitiated reactions at gas-solid interfaces (in collaboration with Professor Curt Wittig): Interactions of vibrationally excited molecules with oxide surfaces are monitored state-selectively with a variety of laser spectroscopies and using high-resolution OPO's. Other collaborative projects are also encouraged.

Interested candidates with prior experience in laser techniques should send their resume and two letters of reference to: Professor Hanna Reisler, Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482; E-mail: [Reisler@chem1.usc.edu](mailto:Reisler@chem1.usc.edu); FAX: (213) 746-4945.

### **POSTDOCTORAL POSITION, University of Notre Dame**

A postdoctoral position is available in the Hammes-Schiffer research group in the general area of reaction dynamics in complex systems. Projects of interest include:

1. Extensions and applications of the TDSCF-RPH (time-dependent self-consistent-field reaction path Hamiltonian) method (see J. Chem. Phys. 108, 7085 (1998) for more information on this topic).
2. Development and applications of mixed quantum/classical molecular dynamics methods, particularly to proton and hydride transfer reactions and photoexcited reactions in solution and in enzymes.
3. Investigation of solvation dynamics of fundamental organic reactions.

Computer programming experience and a strong background in physical chemistry and chemical physics are required. Funding for this position is available immediately, but the starting date is flexible. The expectation is that the position will be for two years, subject to renewal upon mutual agreement after the first year.

See my web site <http://www.nd.edu/~shammes> for more information.

Please send CV and at least 2 letters of recommendation to Professor Sharon Hammes-Schiffer, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, (219) 631-7434,

### **POSTDOCTORAL POSITION, Rice University**

A postdoctoral research position for experimental studies of fullerene photophysics is currently available in the group of Prof. Bruce Weisman at Rice University. The research will focus on using time-resolved spectroscopy to explore triplet state properties and processes in fullerenes and related systems of basic and

applied interest. Motivated applicants with a background in optical methods, kinetic analysis, or fullerenes are preferred. To apply, please send a cover letter, CV, and arrange for three letters of recommendation to: Prof. R. Bruce Weisman, Department of Chemistry, MS-60, Rice University, 6100 Main Street, Houston, TX 77005.

e-mail inquiries are welcome at [weisman@rice.edu](mailto:weisman@rice.edu) Rice University is an Equal Opportunity / Affirmative Action Employer.

#### **POSTDOCTORAL POSITIONS, Weizmann Institute**

Post-doctoral positions in the field experimental "Coherent Control of Chemical Reactions" have become available in the group of Professor Moshe Shapiro at the Weizmann Institute of Science, Rehovot, Israel. The positions are available within the framework of a center of excellence in Coherence Chemistry at the Weizmann Institute and The Hebrew University, and the German-Israeli DIP project in collaboration with Prof. D. Zajfman of the Physics department at the Weizmann Institute.

The experimental work will focus on 2-photon vs. 2-photon phase control of dissociation processes, in continuation of our past demonstration of laser control of electronic degrees of freedom in the Na<sub>2</sub> dissociation process (Phys. Rev. Letters 76: 2886 (1996)).

The candidates will be encouraged (as an option) to also participate in our theoretical work in the topics of: coherent control of chiral synthesis; laser cooling of molecules and laser induced recombination; wavepacket and potential imaging by femtosecond spectroscopy.

Additional details about the group, its activities, and two sample papers, can be found at

<http://chemphys.weizmann.ac.il/~shapiro/home.html>

Interested applicants should contact (electronic mail is preferable): Professor Moshe Shapiro, Department of Chemical Physics, The Weizmann Institute, Rehovot, 76100, Israel

[cfshapir@weizmann.ac.il](mailto:cfshapir@weizmann.ac.il), fax:+972-8-9344123

#### **POSTDOCTORAL POSITION, University of Utah**

A post-doctoral position in the field of molecular dynamics simulations of high-energy and elastomeric materials will be available beginning 1 September 1998. The position will involve development of *ab initio* based potential functions as well as calculation of structural, transport, thermodynamic and mechanical properties of bulk materials and materials interfaces. Efforts will involve algorithm and code development for application on massively parallel platforms. Applicants should have a background in statistical mechanics, molecular dynamics simulations, and code development in FORTRAN. Interested parties should contact Grant D. Smith or Richard H. Boyd, Department of Materials Science and Engineering and Department of Chemical Engineering, University of Utah, Salt Lake City, UT 84112

[gsmith@geoffrey.emro.utah.edu](mailto:gsmith@geoffrey.emro.utah.edu), [boyd@poly2.mse.utah.edu](mailto:boyd@poly2.mse.utah.edu)

#### **POSTDOCTORAL POSITION, University of Lille**

A postdoctoral position in the field "Heterogeneous chemistry of atmospheric radicals" is available in the group of Pr Jean-Pierre Sawerysyn at the University of Lille (France). The project is focused on the heterogeneous chemistry of XO radicals (X= Br, I) on different solid surfaces of atmospheric aerosol materials. Experiments will be performed using a flow tube combined with a molecular beam mass spectrometric sampling technique as a detection method. Furthermore, the applicant will participate to the development of a new technique for investigating the heterogenous chemistry of atmospheric species on liquid surfaces. Duration : Septembre 98 - July 99 (with possible extension). Interested applicants should send a cv and two letters of recommendations to Jean-Pierre Sawerysyn . E-mail will be fine.

LC3-Laboratoire de Cinétique et Chimie de la Combustion, URA CNRS 876- Université des Sciences et Technologies de LILLE, 59655 VILLENEUVE d'ASCQ Cedex.FRANCE.

email : [Jean-Pierre.Sawerysyn@univ-lille1.fr](mailto:Jean-Pierre.Sawerysyn@univ-lille1.fr), T: 33.(0)3.20.43.65.62 Fax : 33.(0)3.20.43.69.77

### **POSTDOCTORAL POSITION, Hebrew University of Jerusalem**

A postdoctoral position is open at the Physical Chemistry department in the Hebrew University of Jerusalem, in the group of Dr. Uri Banin. The topic of research is size dependent spectroscopy and microscopy of semiconductor nanocrystals, and semiconductor cluster-molecules. The successful applicant, should have background and experience in experimental optical spectroscopy of molecules, single molecules or materials, and interest in nanomaterials. The project is a collaboration with a group at the University of Karlsruhe in Germany, and some travel is planned along the course of the work.

Interested parties can contact Dr. Uri Banin, preferably by Email at: [banin@chem.ch.huji.ac.il](mailto:banin@chem.ch.huji.ac.il)

Dr. Uri Banin, Department of Physical Chemistry, The Hebrew University Of Jerusalem, Jerusalem 91904, Israel, TEL.:972-2-6584515, FAX: 972-2-5618033,

<http://chem.ch.huji.ac.il/employee/banin/ibanin.htm>

### **POSTDOCTORAL POSITIONS, Hanscom Air Force Base**

There are two postdoctoral research positions available in the area of laboratory studies of chemical and physical processes of the upper atmosphere, located at the U.S. Air Force Research Laboratory at Hanscom Air Force Base, near Boston, Massachusetts. The research is conducted in an academic style and results are published in the open literature. However, there is a requirement that the candidate be a U.S. Citizen or Permanent Resident (with a "green card").

We have a Laboratory Scholar Program with an immediate opening, and an NRC Research Associateship Opportunity (number 13.03.24.09) that has an August 15, 1998 application deadline.

Our group performs experiments, develops models, and analyzes field measurements relating to the molecular dynamics and infrared spectra of the upper atmosphere. In our laboratory experiments we measure the rates of formation, excitation and deactivation of infrared-active species, especially in highly vibrationally and rotationally excited states. A unique cryogenic simulation chamber is available for these measurements, in which pulsed laser and electron-beam excitation methods are applied, and infrared emissions are studied in an environment in which the background is effectively suppressed. Advanced infrared detection systems used in this work include Michelson interferometers with high resolution and sensitivity. The data obtained using time-resolved Fourier transform spectroscopy are analyzed using techniques such as nonlinear synthetic spectral fitting and spectral pattern recognition algorithms. For example, we are studying the chemical production of OH radicals in states with high  $\nu$  and high N, responsible for pure rotation emissions observed in the atmosphere. We also conduct related laser-based experiments that make use of multiphoton ionization and laser-induced fluorescence to determine state-to-state kinetic properties of a number of species. The results of the laboratory experiments can be analyzed together with the data acquired in rocket-based, Space Shuttle, and satellite experiments, as well as with data from imaging spectrometers. Access to the field measurement data enhances our ability to develop new atmospheric models of the chemically active species we study. The modeled kinetic and radiative processes relate to the energy pathways, temperature structure, and infrared properties of the upper atmosphere.

Please contact Dr. Steve Lipson, U.S. Air Force Research Laboratory (AFRL/VSBM), Hanscom AFB, Massachusetts 01731, Voice (781) 377-3626; Fax (781) 377-8900, E-mail [lipson@plh.af.mil](mailto:lipson@plh.af.mil)

### **POSTDOCTORAL POSITION, University of California, Davis, CA**

A postdoctoral position is available in my research group to study photoexcited triplet states of biomolecules using ODMR (optically detected magnetic resonance) spectroscopy. A major focus is the NIH-funded investigation of retroviral nucleocapsid protein (NC) binding to nucleic acids. Among the NC proteins actively being studied is NCp7 of HIV-1 and its complexes with various elements of the psi-recognition region of its RNA genome. All retrovirus (except spumavirus) NC proteins incorporate one or two essential CCHC-type zinc-finger sequences that contain highly conserved aromatic amino acids such as tryptophan.

These serve as intrinsic spectroscopic probes for ODMR. Retroviral zinc-fingers are promising new targets for attack by antiviral agents that are being studied in a number of laboratories. We maintain active collaborations with biological research groups that provide us with protein and nucleic acid samples. Further information can be found at <http://www-chem.ucdavis.edu/people/maki.html>. If you are interested in being considered for this position please submit a curriculum vitae and the names of three references to Prof. August H. Maki, Department of Chemistry, University of California, Davis, CA 95616, USA.

#### **POSTDOCTORAL POSITION, Columbia University**

I am seeking a postdoctoral researcher for my surface group at Columbia University. The experiments involve energy-resolved measurements of photoreaction of organic molecules on UHV prepared surfaces of metal oxide and/or semiconductor crystal. The work involves mass spectroscopic detection and/or UV REMPI. The goals are the fundamental chemical physics of light-induced single-crystal surface reactions, but on surfaces with environmental and/or electronic implications. Experience in excimer/dye laser technology and REMPI required; experience in UHV methods and computer control required. Good communication skills essential. Please send resumes to Prof. Richard Osgood, Dept. of Electrical Engineering, 500 West 120th Street, rm. 1322, New York, NY 10027, or send to email address: [osgood@columbia.edu](mailto:osgood@columbia.edu). Columbia University is an equal opportunity employer.

#### **POSTDOCTORAL POSITION, University of Illinois at Chicago**

A post-doctoral position is open in the group of Prof. Robert Gordon at the University of Illinois at Chicago in the areas of coherent control and molecular optics. The research associate may work on either of two projects (or both!). The first project is a continuation of ongoing work described in recent publications in *Science* (270, 77 (1995)) and *Physical Review Letters* (79, 4108 (1997)), in which we demonstrated coherent phase control over the branching between ionization and dissociation of HI and DI. Future experiments will include bond-selective photochemistry and control over the angular distributions of photofragments. A recently completed photofragment imaging machine will be used for some of these experiments. In the second project a tightly focused laser beam will be used to create a "molecular lens" that is capable of focusing and steering a molecular beam. Possible experiments include using the focused molecular beam to create nanostructures on a surface and measurement of the alignment of pendular states using a femtosecond probe.

Candidates for this position should have experience with dye lasers, pulsed molecular beams, and ion optics. The position is open now, and funding is available for more than one year. Please send resumes and arrange for letters of recommendation to be sent to Robert Gordon, Department of Chemistry (m/c 111), University of Illinois at Chicago, 845 W Taylor Street, Chicago, IL 60607-7061.

#### **POSTDOCTORAL POSITION IN THEORETICAL CHEMISTRY, Indiana University**

A postdoctoral position is available in my group. The research involves combining techniques from statistical mechanics and electronic structure to solve realistic models of chemical systems via computer simulation. Problems of interest range from electron solvation, to the properties of biopolymers to quantum effects in cryogenic systems. The starting date is flexible and the position will be for one year, with yearly extensions possible. Resumes consisting of a CV, a publication list and the address/phone number/email of two references, may be sent to me by either mail or email.

Professor Glenn J. Martyna, Department of Chemistry, Indiana University, Bloomington, IN 47405-4001, Phone: (812)-855-6605, Fax:(812)-855-8300, Email: [martyna@martyna1.chem.indiana.edu](mailto:martyna@martyna1.chem.indiana.edu)

#### **POSTDOCTORAL POSITION, University of California, Los Angeles**

We are looking for creative and self driven individuals to contribute to our rapidly growing research program in COMBINATORIAL CATALYSIS. Specifically we are looking for expertise in LASER SPECTROSCOPY, someone with good experimental skills and preferably experience in single and multi

color REMPI, laser fragmentation spectroscopy, time of flight mass spectrometry and Labview. REMPI microelectrode technique has recently been developed in our laboratories to rapidly screen large solid state catalyst libraries (see the upcoming July 23 issue of NATURE). Molecules of initial interest are organics, organometallics and metals. We currently have an excimer pumped dye laser system and a TOF mass spectrometer. We are also acquiring a tunable solid state laser (OPO). The candidate is expected to develop laser based ionization/detection schemes to screen gaseous products from solid state catalyst libraries and contribute to the development of a new and exciting field in catalysis. We offer a competitive salary and benefits. Position is available immediately. Please send cv, names of 2-3 references to the address below. If you use e.mail, please send all correspondence in ASCII. Selim M. Senkan, Professor and Chairman, Department of Chemical Engineering, 5531 Boelter Hall, University of California, Los Angeles, CA 90095  
Office Tel: 310-206-4106, Dept. Fax : 310-206-4107, E.Mail: senkan@seas.ucla.edu,  
<http://www.chemeng.ucla.edu>

### **POSTDOCTORAL POSITIONS IN THEORETICAL CHEMISTRY**

Two postdoctoral positions are available in my group. The research involves combining techniques from statistical mechanics and electronic structure to solve realistic models of chemical systems via computer simulation. Problems of interest range from electron solvation, to the properties of biopolymers to quantum effects in cryogenic systems. The starting date is flexible and the position will be for one year, with yearly extensions possible. Resumes consisting of a CV, a publication list and the address/phone number/email of two references, may be sent to me by either mail or email.

Professor Glenn J. Martyna, Department of Chemistry, Indiana University, Bloomington, IN 47405-4001, Phone: (812)-855-6605, Fax: (812)-855-8300, Email: martyna@martyna1.chem.indiana.edu.

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

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

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

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

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

### **POSTDOCTORAL POSITION, UNIVERSITY of MONTREAL**

A postdoctoral position is available in the group of Tucker Carrington Jr. at the University of Montreal, Canada The initial appointment will be for one year but funds are available for a second year. Candidates

should have training in either theoretical chemistry or theoretical physics. Experience in quantum dynamics calculations would be an asset.

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

Interested candidates should send a C.V. and a summary of research interests to Professor Tucker Carrington Jr., Departement de chimie, Universite de Montreal, Case postale 6128, succursale Centre-ville, Montreal (Quebec) H3C 3J7, Canada

tel: (514) 343-2123, fax: (514) 343-7586, e-mail: Tucker.Carrington@umontreal.ca

### **POSTDOCTORAL POSITIONS IN MOLECULAR LASER SPECTROSCOPY AND CHEMICAL KINETICS**

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

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

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

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

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

Phone: (601)-325-0499 (Office); (601)-325-9039 (Lab); Fax: (601)-325-8465; E-mail: vasudev@dial.msstate.edu

### **POSTDOCTORAL POSITIONS, University of Liverpool**

Two post-doctoral research positions are available, one on Theory and one Experimental, to study the dynamics of dissociation at heterogeneous surfaces at the Surface Science Research Centre, University of Liverpool. This project will combine theoretical modelling techniques with detailed state resolved experiments to investigate the influence of coadsorbates on the poisoning and promotion of reactions at well defined metal surfaces.

The experimental position will employ laser detection and molecular beam techniques to investigate

dissociation and recombinative desorption of small molecules at metal surfaces in the presence of a coadsorbate. Applicants should have experience of either UHV surface science techniques or of laser spectroscopy/molecular reaction dynamics.

The theoretical position will involve quantum and classical dynamics simulations of molecular dissociation and scattering; applicants should have experience in a related area.

Further information can be obtained from Dr Andrew Hodgson (Experimental) (0151-794-3536, email: ahodgson@liv.ac.uk) or Professor Stephen Holloway (Theory) (0151-794-3537, email: stephen@ssci.liv.ac.uk). Appointment to this position will be according to age and experience. Applicants should send a cv, together with the names of three referees, directly to us or to the Registrar, University of Liverpool, PO Box 147, Liverpool L69 3BX, UK.

Andrew Hodgson (andrewh@ssci.liv.ac.uk), Surface Science Research Centre, University of Liverpool, P.O. Box 147, Liverpool L69 3BX, UK, Tel: 0151-794 3536, FAX: 0151-708 0662,

### **POSTDOCTORAL POSITION, University of Manchester**

New Theories of Chemical Reactions and Molecular Collisions

Applications are invited for a postdoctoral research associate position funded by the UK Engineering and Physical Sciences Research Council. The research involves the development of novel theories for understanding the dynamics of chemical reactions and molecular collisions. There are two complementary themes to the research:

(a) the dynamics of light atom transfer reactions, which involves computationally intensive scattering calculations. (b) new semiclassical theories for understanding the angular scattering of reactive and inelastic collisions.

Examples of our recent research include: J. Chem. Phys. 1998 (108) 5695; *ibid.* 1996 (104) 2297; J. Chem. Soc. Faraday Trans. 1997 (93) 709; J. Comput. Appl. Math. 1997 (82) 447; Chem. Phys. 1996 (207) 461.

Excellent computational facilities are available for the research including supercomputers and workstations. The research on the dynamics of light atom transfer reactions involves collaboration with Professor G C Schatz, Dept. of Chemistry, Northwestern University, Evanston, Illinois, USA, and some travel to the USA is possible.

The appointment is for 2 years. Salary in the range 15159-22785 UK pounds plus membership of the Universities Superannuation Scheme.

Candidates with strengths in either of the above themes (or both) should send their curriculum vitae and names of two referees to:

Professor J.N.L. Connor, Department of Chemistry, University of Manchester, Manchester M13 9PL, England, Tel: (+44)-161-275-4693/4686, Fax: (+44)-161-275-4734, Email: J.N.L.Connor@Manchester.ac.uk

### **POSTDOCTORAL POSITION, Australian National University**

A postdoctoral position will probably be open in our chemical dynamics group from later this year. Our group is interested in a number of aspects of molecular motion and chemical reaction dynamics. The successful candidate will be expected to work on the development of methods for constructing molecular potential energy surfaces [see our recent advances in, for example, JCP 102, 5647 (1995); 108, 2424 (1998), 108, 8302 (1998); and J. Chem. Soc. Far. Trans. 93, 871 (1997)].

For this position, some experience with *ab initio* calculations might be useful, but is not essential. Interested applicants should have high quality theoretical ability.

The position is for two years in the first instance, with the possibility of extension to a third year.

Interested candidates are asked to send me a brief Curriculum Vitae and list of publications, via email (collins@rsc.anu.edu.au), or Fax (61 6 249 0750).

Unfortunately, time is short, so interested candidates are asked to contact me as soon as possible, and no later

than August 20, 1998. Dr Michael A. Collins, Research School of Chemistry, Australian National University, Canberra. ACT. 0200, Australia

#### **POSTDOCTORAL POSITION, Rice University**

Robert F. Curl and Graham P. Glass of the Chemistry Department at Rice University are seeking a Post-doctoral Fellow in the field of infrared laser kinetic spectroscopy of free radicals. In these experiments, a suitable precursor for the radical of interest is flash photolyzed by an excimer laser and the transient infrared absorption of radical produced is observed using a tunable, cw IR laser probe. The probe lasers are a color center laser and a difference frequency source. For somewhat more information see <http://pchem1.rice.edu/FacultyStaff/Curl.html> and its linked page. This position requires extensive experience with lasers and the normal technology of Chemical Physics. Previous experience working with cw tunable lasers preferably Coherent Autoscan Ti:sapphire lasers is desirable. The position is restricted to individuals who have received their doctorates within the last five years. Please send a resume and arrange for two letters of recommendation to be sent to Robert Curl, Chemistry Department, Rice University, Houston, TX 77005-1892, USA ([rfcurl@rice.edu](mailto:rfcurl@rice.edu)) by August 15, 1998. Rice University is an Affirmative Action/Equal Opportunity Employer.

#### **POSTDOCTORAL POSITION, Cambridge University**

There are two major problems in extrapolating data obtained under ultrahigh vacuum (uhv) conditions, using surface science methods, to the study of catalysts under realistic conditions. These problems are commonly referred to as the "structure gap" and the "pressure gap", reflecting the differences in surface structure and ambient pressure, respectively, between practical catalysts operated at elevated pressures and single crystal surfaces studied under uhv conditions.

The aim of this project is to bridge these gaps by using new laser spectroscopic methods that can be used to study the adsorbed species present on the surface of a working single crystal model catalyst in the appropriate reactive atmosphere and at the relevant temperature. Second harmonic generation spectroscopy and sum frequency generation spectroscopy provide us with powerful in situ tools for investigating the structure of the catalyst surface and the vibrational spectra of chemisorbed molecules under reaction conditions.

A postdoctoral position is available for two years in the research group of Dr David Klenerman in the Department of Chemistry, Cambridge University, commencing as soon as possible. Applicants should have a background in laser spectroscopy and some vacuum experience would be useful. The instrumentation required to carry out the project has already been built and successfully tested, including a state-of-the-art tunable picosecond infra-red laser source and uhv and high pressure cells. Our principal objective is to exploit these new methods in the investigation and development of technologically important catalytic systems. To apply please send a CV and the name of two referees to :

Dr. David Klenerman, Department of Chemistry, University of Cambridge, Lensfield Road, CAMBRIDGE CB2 1EW, Tel: 44-1223 336481, fax: 44-1223-336362, email: [dk10012@cam.ac.uk](mailto:dk10012@cam.ac.uk).

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

#### **POSTDOCTORAL POSITION, HEBREW UNIVERSITY OF JERUSALEM**

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

The research focuses on developing novel theoretical models and numerical methods to study the properties of very large atomic and molecular systems. Specifically, much research will be devoted to developing linear

scaling methods for electronic structure and will include the incorporation of the new ideas and techniques into a fast Kohn-Sham DFT code.

Recent developments we have made can be found in: <http://chem.ch.huji.ac.il/employee/baerr/ibaerr.htm>. Starting date is flexible -end of this year or beginning of next. Please send curriculum vitae and the names of three references to: Dr. Roi Baer, Dept. of Physical Chemistry, Hebrew University, Jerusalem 91904, Israel or via email to [roib@fh.huji.ac.il](mailto:roib@fh.huji.ac.il).

### **POSTDOCTORAL POSITION IN ATMOSPHERIC PHYSICAL CHEMISTRY**

Candidates are sought for a postdoctoral position at the University of Chicago in the field of atmospheric physical chemistry. Funded by a prestigious award from the Camille and Henry Dreyfus Foundation, this position provides an opportunity for outstanding chemists to perform research in environmental science. The salary set by the Dreyfus Foundation is \$35,000/yr. The visiting scientist will work in the laboratories of Prof's. L. Butler and/or J. Abbatt, in a program designed jointly with the visiting scientist to maximize his/her ease of entree into this interdisciplinary area. Potential projects include: photochemistry of atmospheric species, the optical properties of aerosols, and atmospheric heterogeneous chemistry. Candidates should send a cv, letter of research interests, and the names and addresses of three potential references to either Prof. L. J. Butler, James Franck Institute and Dept. of Chemistry, The University of Chicago, 5640 S. Ellis Ave., Chicago, IL, 60637 or Prof. J. Abbatt, Dept. of the Geophysical Sciences, The University of Chicago, 5734 S. Ellis Ave., Chicago, IL, 60637, by Sept. 30, 1998.  
<http://geosci.uchicago.edu/Faculty/ABBATT/abbatt.html>  
<http://rainbow.uchicago.edu/chemistry/fac/butler.html>

## **b. Preprints**

### **Creation and Manipulation of Coherences in Molecules with a Pulse Magnetic Field**

European Journal of Physics D

H. Ring, R. T. Carter and J. R. Huber\*

Physical Chemistry Institute, University of Zurich, Winterthurerstr. 190, CH-8057 Zurich, Switzerland

We demonstrate the application of a pulsed magnetic field for the creation and manipulation of coherences in molecular systems, using quantum beat spectroscopy for the detection of the dynamics of the molecular superposition states.

### **Theoretical Treatment of Surface Adsorbates**

Computational Studies of New Materials Edited by D. A. Jelski and T. F. George (World Scientific, Singapore, 1998)

L. Nanai, C. Beleznai and Thomas F. George\*

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

Theoretical and computational methods used to describe chemisorption and adsorbate reactions on solids, mainly metallic surfaces, are reviewed.

### **Quantum Correspondence for Linear Canonical Transformations on General Hamiltonian Systems**

Physical Review A

Kyu Hwang Yeon, Dan F. Wallis, Chung-In Um, Thomas F. George\*, and Lakshmi N. Pandey

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

General Hamiltonian systems related by linear canonical transformations, which are combinations of the scale and gauge transformations, are considered with the help of path integrals.

### **Ground-State Properties of Two-Dimensional $^3\text{He}$ - $^4\text{He}$ Mixtures: Energetics and Structures**

Journal of Low Temperature Physics

Chung-In Um, Jaei-Rok Kahng and Thomas F. George\*

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

A variational Jastrow wavefunction extended to include a three-body correlation function and a hypernetted and Fermi hypernetted chain scheme with contribution from elementary diagrams is used to analyze ground-state energies and structural properties of two-dimensional  $^3\text{He}$ - $^4\text{He}$  mixtures.

### **A New Scheme to Calculate Dipole-Allowed Singlets in Conjugated Polymers**

Journal of Chemical Physics

G. P. Zhang, Thomas F. George\*, and Lakshmi N. Pandey

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

Properly combined with the Lanczos interaction algorithm, the density matrix renormalization group is used to directly calculate the dipole-allowed singlet states and the transition moment elements between these states and the ground state for long chains.

### **Production of the molecular dication $\text{ArN}^{2+}$ in the reaction $\text{Ar}^{2+} + \text{N}_2$**

P.Tosi, R. Correale, W. Lu, S. Falcinelli, D.Bassi

Istituto Nazionale per la Fisica della Materia and Dipartimento di Fisica  
Universita' di Trento, I-38050 Povo, Italy

### **Production of $\text{ArN}^+$ ions in the reactions $\text{Ar}^+ + \text{N}_2$ and $\text{N}_2^+ + \text{Ar}$**

P.Tosi, R.Correale, W.Lu, D.Bassi

Istituto Nazionale per la Fisica della Materia and Dipartimento di Fisica  
Universita' di Trento, I-38050 Povo, Italy

### **The He-LiH potential energy surface revisited. I. An interpolated rigid rotor surface**

J. Chem. Phys., submitted

Brian K. Taylor and Robert J. Hinde\*

Department of Chemistry, University of Tennessee Knoxville, Tennessee 37996-1600, U.S.A.

We reconsider the potential energy surface of the He-LiH system recently examined by Gianturco and co-workers [F. A. Gianturco et al., Chem. Phys. 215, 227 (1997)]. We compute the He-LiH interaction energy at the CCSD(T) level using large correlation consistent atomic basis sets supplemented with bond functions. Our potential surface differs substantially from that of Gianturco et al.; in particular, our attractive He-LiH well is more than twice as deep as that of Gianturco et al., with a He-LiH binding energy of 176.7 wavenumbers.

### **First quantum investigation of the photodissociation of the Ar-HBr complex: three-dimensional time-dependent approach.**

Chemical Physics Letters

M. Monnerville\*, B. Pouilly

Laboratoire de Physique des Lasers, Atomes et Molécules, Université des Sciences et Technologies de Lille I  
59655 Villeneuve d'Ascq Cedex, France

The ultraviolet photodissociation of the Ar-HBr van der Waals complex is studied using an exact three-dimensional time-dependent wavepacket approach with zero-total angular momentum.

### **New investigation of the photodissociation of the HBr molecule: total cross section, anisotropy parameter and dependence of the spin-orbit branching on the ground state vibrational level**

Chemical Physics Letters

M. Monnerville\*, B. Pouilly

Laboratoire de Physique des Lasers, Atomes et Molécules, Université des Sciences et Technologies de Lille I

59655 Villeneuve d'Ascq Cedex, France

New calculations on the photodissociation of the HBr molecule in a time-independent framework are reported. Dependence on excitation wavelength of both the total cross section and the anisotropy parameter have been calculated as well as dependence of the spin-orbit branching ratio on the initial vibrational level.

### **The hyperpolarisability of an endohedral fullerene: Li@C<sub>60</sub>**

Chem. Phys. Lett. 288 (1998) 131-137

E. E. B. Campbell, M. Fanti+, I. V. Hertel, R. Mitzner\* and F. Zerbetto

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

+Istituto di Spettroscopia Molecolare, Consiglio Nazionale delle Ricerche, Via Gobetti 101, Bologna, Italy

Dipartimento di Chimica "G. Ciamician", Università degli Studi di Bologna, Via F. Selmi 2, 40126 Bologna, Italy

A sum over molecular orbitals scheme with an ab initio 6-31G\* basis set is used to calculate the static first hyperpolarisabilities, of Li@C<sub>60</sub>, an endohedral derivative of C<sub>60</sub>, recently synthesised in sizeable quantities. In the most stable form, that is when the Li atom is ~1.5 Å off the centre of the cage, the calculated  $\beta$  is comparable to that of the best organic materials and to that of push-pull fullerenes to-be-synthesised. Because of the orbiting character of the motion of Li inside the carbon cage, and the substantial variation of the hyperpolarisability with the location of the Li atom, it is suggested that the  $\chi^{(2)}$  of this material will: a) be between one and two orders of magnitude larger than the magnetically induced  $\chi^{(2)}$  of pristine C<sub>60</sub>; and b) show a strong temperature dependence. Comparison with preliminary measurements shows satisfactory agreement.

### **Decay of the ammonia B state due to nonadiabatic coupling**

Chem. Phys. Lett. 289 (1998) 46-52

H.-H. Ritze, W. Radloff and I. V. Hertel

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

In real-time two-colour pump-probe ionization experiments of NH<sub>3</sub> and ND<sub>3</sub> using femtosecond 155 nm excitation pulses the lifetime of several vibronic B levels was measured. The results obtained are discussed in terms of a simple model of nonadiabatic coupling between B and A vibronic levels.

### **Temporal coherent control induced by wave packet interferences on one and two photon atomic transitions**

The European Physical Journal D 2 (1998) 131-141

M. A. Bouchene, V. Blanchet, C. Nicole, N. Melikechi, B. Girard, H. Ruppe\*, S. Rutz\*, E. Schreiber\*, and L. Wöste\*

Laboratoire des Collisions Agrégats Réactifs, C.N.R.S., IRSAMC, Université Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse Cedex, France

Freie Universität Berlin, Experimentalphysik, Arnimallee 14, 14169 Berlin, Germany

The interaction of a sequence of two identical ultrashort laser pulses with an atomic system results in quantum interferences as in Ramsey fringes experiments. These interferences allow achievement of temporal coherent control of the excitation probability. We present the results of a temporal coherent control experiment on two different atomic systems: one-photon absorption in K (4s-4p) and two-photon absorption in Cs (6s-7d). In K, the quantum interferences between the two excitation paths associated with the laser pulses are revealed through rapid oscillations of the excitation probability as a function of the time delay between the two pulses.

### **Ultrafast photodissociation dynamics of electronically excited CF<sub>2</sub>I<sub>2</sub> molecules**

Chem. Phys. Lett. 288 (1998) 178-178

W. Radloff+, P. Farmanara+, V. Stert+, E. Schreiber+ and J. R. Huber\*

+Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

Physikalisch-Chemisches Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich,

Switzerland

Using the femtosecond pump-probe technique in combination with REMPI-TOF mass spectrometry we investigated the photodissociation dynamics of  $\text{CF}_2\text{I}_2$ . After excitation by the 267 nm pump pulse (probe pulse 400 nm), a relaxation process with a time constant  $t \simeq 30$  fs leads to an intermediate state of  $\text{CF}_2\text{I}_2$ , which subsequently dissociates with  $t \simeq 100$  fs into  $\text{CF}_2$ , I and  $\text{I}_2$ . Within experimental error ( $\pm 30$  fs) these fragments are formed with the same rate. Since in addition no evidence of a transient species  $\text{CF}_2\text{I}$  was found, a concerted reaction mechanism is proposed for this ultrafast dissociation process.

### **Ultrafast internal conversion and fragmentation in electronically excited $\text{C}_2\text{H}_4$ and $\text{C}_2\text{H}_3\text{Cl}$ molecules**

Chem. Phys. Lett. 288 (1998) 518-522

P. Farmanara, V. Stert, W. Radloff

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

The time constants of internal conversion and fragmentation have been determined for ethylene and vinyl chloride excited by 125 fs laser pulses of the wavelength 200 nm. In  $\text{C}_2\text{H}_4$  the internal conversion from the lowest excited electronic state to the ground state proceeds within  $t_{IC} = 30 \pm 15$  fs. In  $\text{C}_2\text{H}_3\text{Cl}$  the internal conversion with  $t_{IC} = 30 \pm 10$  fs leads to the fast dissociating S1 state ( $t_F = 40 \pm 10$  fs) as well as to the  $\text{S}_0$  ground state which decays within about 110 ps.

### **Effects of excitation and orbital alignment on $\text{Na}^+ + \text{Na}$ electron transfer**

J. Phys. B 31 (1998) 3429-3437

J. W. Thomson, N. Andersen, E. E. B. Campbell\*, I. V. Hertel\* and S. E. Nielsen

Niels Bohr Institute, Orsted Laboratory, Universitetsparken 5, DK-2100 Copenhagen, Denmark

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

Department of Chemistry, H. C. Orsted Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

The effects of excitation and orbital alignment on the electron transfer process in  $\text{Na}^+ - \text{Na}(3s, 3p)$  collisions are investigated experimentally and theoretically over a wide range of impact energies. Experimentally, the  $\text{Na}(3p)$  integral alignment parameter and the ratios between the integral transfer cross sections for  $\text{Na}(3p, 3p)$  targets to that for a  $\text{Na}(3s)$  target have been determined using an optically prepared target. The results are in good agreement with earlier data at lower energies of Campbell et al. Theoretically, the integral cross section results of our 26 state two-centre atomic orbital close-coupling calculations are in good agreement with all experimental data, including the absolute electron transfer cross section measurements of Daley and Perel. These processes are now well understood over more than three orders of magnitude for the impact energy range.

### **Production, HPLC Separation and UV-VIS spectroscopy of $\text{Li}@C_{70}$**

Intern. Winterschool on Electronic, Properties of Novel Materials; eds: H. Kuzmany, J. Fink, Me Mehring and S. Roth; World Scientific (1998)

N. Krawez, A. Gromov, R. Tellgmann and E. E. B. Campbell

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

Endohedral  $\text{Li}_n@C_{70}$  (with  $n = 1, 2, 3$ ) can be produced by low energy ion bombardment of  $C_{70}$  thin films.

Considerably more multiple capture is found for  $C_{70}$  than was the case for  $C_{60}$ . The monomer endohedral species  $\text{Li}@C_{70}$  has been purified by HPLC. Unlike  $C_{60}$ , only one endohedral fraction is found. The UV-VIS spectra of  $\text{Li}@C_{70}$  in  $\text{CS}_2$  and toluene are reported and compared with  $C_{70}$

### **Spectrograms as a Tool to control Laser-Induced Femtosecond Molecular Dynamics**

in Lasers'97, V. J. Corcoran and T. A. Goldman eds. (Soc. of Opt. and Quant. El., McLean, USA (1998) 270-276

E. Schreiber

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

The application of the spectrogram technique to the ultrafast spectroscopy of molecules is demonstrated. It is shown, how spectrograms enable deeper insight into the femtosecond molecular dynamics induced by sub- 100 fs laser pulses. The potassium dimer, excited to its electronic A state, is a prototype molecule for investigations of fundamental wave packet propagation phenomena and acts here as the workhorse. Fascinating total and fractional revivals of the laser-induced wave packet dynamics are observed and analysed by spectrograms.

### **Ultrafast Photoelectron Spectroscopy: Femtosecond Pump-Probe Coincidence Detection of Ammonia Cluster Ions and Electrons**

Journal European Physics D

V. Stert, W. Radloff, C. P. Schulz and I. V. Hertel

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

A new type of experiment is described, in which the femtosecond pump-probe method is combined with the photoelectron-photoion coincidence technique and time of flight photoelectron energy analysis. The experimental conditions for observing true coincidences are discussed. The performance of the new time resolved, ultrafast photoelectron spectroscopy is exemplified by studying the excited state dynamics of ammonia molecules and clusters.

### **Isotope-Selective Femtosecond Wave Packet Dynamics the Rare $41,41, K_2$ Molecule**

The European Physical Journal D

S. Rutz\* and E. Schreiber+

Universitt Rostock, Universittsplatz 3, 18051 Rostock, Germany

+Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

For the first time, the femtosecond real-time vibrational dynamics of the rare  $41,41, K_2$  isotope, excited to the electronic  $A^1\Sigma^+$  state, could be selectively studied by means of time-resolved three photon ionization. A vibrational period of  $T_A(41,41)$  @ 500 fs is determined. Superimposed, a beat structure with a period of 20 ps is observed. A detailed Fourier analysis reveals a strong band of three lines centered around  $65,5 \text{ cm}^{-1}$ .

### **Growth of carbon nanotubes by fullerene decomposition in the presence of transition metals**

Chem. Phys. Lett. submitted

L. P. Biro\*, R. Ehlich\*, R. Tellgmann\*, A. Gromov\*, N. Krawez\*, M. Tschaplyguine\*, M.-M. Pohl<sup>+</sup>, E. Zsoldos#, Z. Vrtessy#, Zs. Horvth# and E. E. B. Campbell\*+

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

<sup>+</sup>Institut fr Angewandte Chemie, Rudower Chaussee 5, D-12489 Berlin, Germany

#MFA, Research Institute for Technical Physics and Materials Science, H-1525 Budapest, P.O. Box 49, Hungary

+Now at School of Physics and Engineering Physics, Gothenburg University and Chalmers University of Technology, S-41296 Gothenburg, Sweden

Carbon nanotubes are formed on HOPG from  $C_{60}$  sublimed from a stainless steel oven at 450 C. No nanotubes were found on gold under the same conditions or when a quartz oven was used for sublimation. Interesting conical nanostructures are found in the insoluble residue from the stainless steel oven. We interpret the nanotube formation to be due to the presence of small carbon fragments produced by the catalytic decomposition of  $C_{60}$  in the oven.

### **Capture Dynamics in Collisions between Fullerene Ions and Rare Gas Atoms**

Chem. Phys. submitted

E. E. B. Campbell+, R. Ehlich\*, G. Heusler\*, O. Knospe, H. Sprang\*

+School of Physics and Engineering Physics, Gothenburg University and Chalmers University of Technology, S-41296 Gothenburg, Sweden

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

Institut fr Theoretische Physik, Technische Universitt Dresden, D-01062 Dresden, Germany

+present address: Peoplesoft, Mnchen, Germany

The collision energy dependence of capture in collisions between  $C_{60}^+$  ions and small rare gas atoms (He, Ne) is studied in detail and compared with the results of classical molecular dynamics simulations. Additional insight is obtained on the dynamics of the collisions by also studying the kinetic energy loss of the projectile ions. Two capture mechanisms are found for He collisions: penetration of a six-membered ring with no significant cage distortion and scattering from a  $C_{60}$  unit followed by deflection inside the cage.

### **Electronically excited states in size selected solvated alkali metal atoms III: Depletion spectroscopy of $Na(NH_3)_n$ -Clusters**

J. Chem. Phys., submitted

P. Brockhaus\*, I. V. Hertel+ and C. P. Schulz+

+Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany

present Address: University of Southern California, Department of Physics SSC 300, Los Angeles, CA 90089, USA

The first electronically excited state of small  $Na(NH_3)_n$  clusters up to  $n = 22$  is studied by means of depletion spectroscopy. A drastic decrease of the excitation energy from the  $3s \rightarrow 3p$  transition of the Na-atom ( $16950 \text{ cm}^{-1}$ ) down to  $6000 \text{ cm}^{-1}$  for the  $Na(NH_3)_4$  cluster, the closing of the first solvation shell, is observed. For larger clusters the excitation energy increases slightly towards the bulk value ( $6300 \text{ cm}^{-1}$ ) which represents the absorption of the "solvated" electron. For all  $Na(NH_3)_n$  clusters with  $n \geq 3$  a strong absorption peak is observed near  $6600 \text{ cm}^{-1}$ . By comparison with deuterated sodium-ammonia clusters this absorption can be assigned to an intramolecular vibrational overtone of the ammonia molecule. This indicates a strong coupling between electronic and vibrational excitation in the  $Na(NH_3)_n$  clusters

## **c. Conferences**

### **1. WORKSHOP ON ELECTRON TRANSMISSION THROUGH MOLECULES AND MOLECULAR INTERFACES**

Maagan, Sea of the Galilee, Israel, December 13-17, 1998

Organizers:

Ron Naaman, Department of Chemical Physics, Weizmann Institute of Science, 76100 Rehovot, Israel, Phone 972 89342367, Fax 972 89344123, email: cinaaman@wis.weizmann.ac.il

Abraham Nitzan, School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel, Phone 972 36408904, Fax 972 364089293, email: nitzan@chemib4.tau.ac.il

The goal of the workshop is to bring together experimentalists and theoreticians working on the problem of electron transfer and electron transmission at interfaces, giving particular attention to the interrelationship between interface structure and dynamics and its electron transmission properties.

The program will consist of invited and contributed lectures and a poster presentation

List of Invited Speakers (provisional)

U. Banin, Jerusalem, I. Benjamin, Santa Cruz, D. Cahen, Rehovot, S. Datta, Purdue, C. Dekker, Delft, Y. Eichen, Haifa, D. Evans, Albuquerque, M. Gratzel, Lausanne, C.B. Harris, Berkeley, I. Hertel, Berlin, Y. Imry, Rehovot, C. Joachim, Toulouse, J. Jortner, Tel Aviv, A.A. Kornyshev, Juelich, A.M. Kuznetsov, Moscow, V. Mujica, Caracas, R. Naaman, Rehovot, A. Nitzan, Tel Aviv, A.J. Nozik, Golden, Co, M. Ratner, Northwestern, Y. Rosenwaks, Tel Aviv, S. Roth, Stuttgart, L. Sanche, Sherbrooke, W. Schmickler, Ulm, U. Sivan, Haifa, N. Ueno, Chiba, D. Waldeck, Pittsburgh, P.S. Weiss, University Park, I. Willner, Jerusalem, M. Wolf, Berlin, A. Yacoby, Rehovot,

CALL FOR PAPERS

Participants are invited to submit abstracts. Abstracts should be submitted either by e-mail or by airmail (on

a plain white paper 21.5x28 cm with 2.5 cm margin on all sides). The entire abstract, including title, authors, affiliations, tables and references, may not exceed one page. Deadline for submission of abstracts is September 15, 1998. Please indicate clearly with each submission the name, complete address including telephone, fax and e-mail of the presenting author.

Send abstracts either by E-mail to: [cinaaman@wis.weizmann.ac.il](mailto:cinaaman@wis.weizmann.ac.il), or by airmail to: Ron Naaman, Department of Chemical Physics, Weizmann Institute of Science, 76100 Rehovot, Israel.

## **2. THE 5th GORDON CONFERENCE ON GAS PHASE ION CHEMISTRY**

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

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

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

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

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

## **3. WORKSHOP ON "TIME-DEPENDENT QUANTUM MOLECULAR DYNAMICS"**

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

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

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

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

## **4. 18<sup>th</sup> International Symposium on Molecular Beams 1999**

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

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

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

## **5. COMET XVI (XVI International Conference on Molecular Energy Transfer)**

Assisi, Italy, 20-25 June, 1999

Piergiorgio Casavecchia (Chair) and Antonio Laganà (Co-Chair).

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

A Web-page is being prepared at the URL address:

<http://www.chm.unipg.it/chimgen/mb/cong/comet.html>

## **6. WORKSHOP ON QUANTUM REACTIVE SCATTERING**

Perugia, Italy, 25-27 June, 1999

The meeting, which will be sponsored by the D9 COST Action in Chemistry, will hopefully be attended by most of the world experts in the field, and will be run in the same spirit and with the same objectives as the four previous workshops on reactive scattering (Cambridge UK, 1990, organised by David Clary, Cambridge USA, 1994, organised by Yan Sun and Michael Baer, Nottingham UK, 1995, organised by David Clary and David Manolopoulos, and Telluride, Colorado, 1997, organised by Joel Bowman).

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

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

## **7. EUROPEAN COMPUTATIONAL CHEMISTRY SCHOOL: MOLECULAR AND REACTION DYNAMICS**

Perugia, Italy, June 28 - July 4, 1999

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

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

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

For further information contact Prof. Antonio Lagana'

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

email lag@unipg.it,

tel. +39.75.5855515, tel. +39.75.5855606.

Information will also appear soon in the web ([www.chm.unipg.it/chimgen/mb/theo1/gicc.html](http://www.chm.unipg.it/chimgen/mb/theo1/gicc.html))

## **8. THE 1999 AMERICAN CONFERENCE ON THEORETICAL CHEMISTRY (ACTC)**

Boulder, June 27-July 2 1999

Information: Prof. Eric Heller

[heller@physics.harvard.edu](mailto:heller@physics.harvard.edu)

## **9. STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS**

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

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

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

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

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

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

- \* Demonstrations of active or coherent control of chemical processes

At this time we are seeking Titles and Abstracts of about 300 words. The DEADLINE for submission of these proposed contributions is FRIDAY 29 MAY 1998. They should be sent to Dr. BJ Whitaker, School of Chemistry, University of Leeds, LS2 9JT and may be in any form - manuscript, fax, whatever but electronic attachments will be particularly cherished. Papers should be concerned with new, unpublished work. The full proceedings of the Discussion will be published late in 1999, but papers accepted for discussion will be circulated to all participants before the meeting in July 1999. Those unfamiliar with the unique format of Faraday Discussions can obtain more information from the URL above.

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

email: benw@chem.leeds.ac.uk, tel: (44) 113 233 6580, fax: (44) 113 233 6565

#### **10. THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE**

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

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

#### **11. ICPEAC XXI**

July 22 - 27, 1999, Sendai, Japan

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

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

This symposium is organized by the IAU working group on Astrochemistry (D.A. Williams (chair); E.F. van Dishoeck (secretary)) and will cover various topics in molecular astrophysics, including Basic molecular processes: gas-phase and gas-grain interactions; Physics and chemistry of star-forming regions: shocks, jets, PDR's and masers; Molecules in circumstellar disks; Solar system connection: comets, meteorites and IDPs; Chemistry in the inner and outer solar nebula; Atmospheres of planets and brown dwarfs; Diffuse and translucent clouds; Molecules and dust formation in circumstellar envelopes around late-type stars. For further information, see <http://www.issa.re.kr/~iau197/>. To receive future mailings, send e-mail to: [iau197@hanul.issa.re.kr](mailto:iau197@hanul.issa.re.kr).

## **Special announcement**

### **TRIBUTE TO MARYVONNE LE DOURNEUF**

After the untimely death of our colleague in the autumn of 1997, many people expressed the desire to hold a scientific colloquium as a tribute to her work and to the important role she played in the atomic and molecular physics community, both nationally and internationally. This colloquium will be held in the "Salle de la Terrasse", CNRS, Gif sur Yvette on the 23 October 1998.

Maryvonne Le Dourneuf pursued her research with passion, equally interested in fundamental physics, the development of new rigorous theoretical methods in order to understand the mechanisms behind various atomic and molecular processes, and to calculate high precision atomic data.

The invited speakers will review past and recent advances in a number of fields to which Maryvonne Le Dourneuf has contributed, in particular the theoretical study of collisional dynamics involving photons, electrons, atoms, ions and molecules. Applications in astrophysics will also be discussed, where the quality of the atomic data is of crucial importance in the modelling of stellar envelopes.

Speakers include: P. G. Burke, L. Vo Ky, W. R. Johnson, B. I. Schneider, A. Huetz, C. Cohen Tannoudji, W. D. Robb, H. E. Saraph, C. J. Zeippen, C. H. Greene, S. Watanabe, J-M. Launay

Please contact:

L. Malegat, LSAI, Universite Paris-Sud, Bat. 350, F-91405 Orsay, France. Tel.: 33 1 69 15 75 03

(international) 01 69 15 75 03 (national). Fax: 33 1 69 15 58 11 (international) 01 69 15 58 11 (national).

e-mail: Laurence.MALEGAT@lsai.u-psud.fr

## **SPECIAL MATERIALS**

### **BOOKS**

New book on Molecular Clusters.

Vol. III of "Advances in Molecular Vibrations and Collision Dynamics", eds. J. M. Bowman and Z. Bacic (JAI, Greenwich, 1998), xi, 460 pp.

Content:

Molecular clusters: real-time dynamics and reactivity, energetics and dynamics of argon-water photodissociation, interactions between CN radicals and rare gases atoms: collisions, clusters and matrices, vibrational spectroscopy of small size-selected clusters, quantum Monte Carlo vibrational analysis and three-body effects in weakly bound clusters, vibration-rotation-tunneling dynamics of the (HF)<sub>2</sub> and (HCl)<sub>2</sub> from full-dimensional quantum bound-state calculations, spectroscopy and quantum dynamics of hydrogen fluoride clusters, the infrared spectroscopy of hydrogen-bonded clusters: chains, cycles, cubes and three-dimensional networks ab initio characterization of water and anion-water clusters, diffusion Monte Carlo studies of water clusters, rearrangements and tunneling in water clusters, spectroscopy and microscopic theory of doped helium clusters.

### **Companion to Angular Momentum**

We are pleased to announce that "Companion to Angular Momentum" by Valeria Kleiman, Robert J. Gordon, Hongkun Park, and Richard N. Zare has been published in North America on August 7, 1998 by John Wiley & Sons, Inc.

Facts about this book: "Companion to Angular Momentum" will contain the complete solutions to all of the problem sets contained in Zare's "Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics." This companion book is intended to aid the reader to overcome difficulties encountered in learning angular momentum theory by supplying detailed illustrations of the solution methods with an emphasis on those aspects that are often not immediately apparent. Step-by-step explanations are provided to save the reader from the large amount of time often needed to fill in missing gaps that are usually found between the

steps of illustrations in textbooks. Corrections are listed for all known errors in the second printing of "Angular Momentum." The book is about 200 pages in length with a 8 1/2 x 11 trim paper cover. Tentative Price: \$ 29.95 U. S. Dollars. ISBN: 0-471-19249-X

Ordering Information: To order this book, you may call Wiley customer service, at 1-800-Call-Wiley; email, [Custserv@Wiley.com](mailto:Custserv@Wiley.com); or visit their website, at <http://www.wiley.com>. You may also contact Terry Dionisio by fax at (212) 850-8888 for more information.

**Modern Methods for Multidimensional Dynamics Computations in Chemistry**

Modern Methods for Multidimensional Dynamics Computations in Chemistry, edited by D. L. Thompson was published by World Scientific, April 1998 (ISBN: 981-02-3342-6).

This volume describes theoretical methods for treating chemical dynamics problems ranging from gas-phase bimolecular reactions to complex processes in condensed phases.

Further information can be obtained from: <http://www.wspc.com.sg>