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## 2002 GORDON RESEARCH CONFERENCE

on Atomic & Molecular Interactions

### FINAL PROGRESS REPORT

DOE

DE-FG-02-02ER15320

The Gordon Research Conference (GRC) on Atomic & Molecular Interactions was held at Roger Williams University, Bristol, Rhode Island, July 7-12, 2002. The conference was well attended with 110 participants (list enclosed). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both US and foreign scientists, senior researchers, young investigators, and students.

In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field (program enclosed).

I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

Albert Wagner  
Conference Chair

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## Atomic & Molecular Interactions

July 7-12, 2002  
Roger Williams University  
Bristol, RI

Chair: Albert Wagner  
Vice-Chair: Paul Dagdigan

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### SUNDAY

- 2:00 pm - 9:00 pm    Arrival and check-in
- 6:00 pm                Dinner
- 7:30 pm - 9:45 pm    **Reaction Dynamics and the Potential Energy Surface: Larger Systems**  
Discussion Leader: **Michael Collins** (Australian National University, Australia)
- 7:30 pm - 8:15 pm    **Donald Truhlar** (University of Minnesota, USA)  
"Potential Energies for Chemical Reactions"
- 8:15 pm - 9:00 pm    **H. Floyd Davis** (Cornell University, USA)  
"Insertion, Abstraction, and Long-Lived Complexes in Bimolecular Chemical Reactions"
- 9:00 pm - 9:45 pm    **Todd Martinez** (University of Illinois, USA)  
"First Principles and Nearly First Principles Nonadiabatic Dynamics"

### MONDAY

- 7:30 am - 8:30 am    Breakfast
- 8:30 am                Photo
- 9:00 am - 12:30 pm   **Reaction Dynamics and the Potential Energy Surface: Smaller Systems**  
Discussion Leader: **Evelyn Goldfield** (Wayne State University, USA)
- 9:00 am - 9:45 am    **Lawrence Harding** (Argonne National Laboratory, USA)  
"Radical-Radical Reactions"
- 9:45 am - 10:30 am   **Craig Taatjes** (Sandia National Laboratory, USA)  
"Kinetic Isotope Effects in Elementary Reaction Kinetics of Combustion Species"
- 10:30 am               Coffee Break
- 11:00 am - 11:45 am   **Joel Bowman** (Emory University, USA)  
"Quantum dynamics of chemical reactions in full and reduced dimensionality"
- 11:45 am - 12:30 pm   **Xueming Yang** (Institute for Atomic and Molecular Sciences, Taiwan)  
"State-to-State Dynamics of Elementary Chemical Reactions"
- 12:30 pm               Lunch
- 1:30 pm - 6:00 pm    Free Time
- 6:00 pm                Dinner
- 7:30 pm - 9:45 pm    **Half-Collision Dynamics and the Potential Energy Surface**  
Discussion Leader: **Reinhard Schinke** (Max-Planck-Institut für Stromungsforschung, Germany)
- 7:30 pm - 8:15 pm    **Andrew Orr-Ewing** (University of Bristol, England)  
"Photofragment alignment and orientation from ion imaging studies of BrCl photodissociation"
- 8:15 pm - 9:00 pm    **Marc van Hemert** (Universiteit Leiden, The Netherlands)  
"Signatures of the Potential Energy Surface from Photodissociation of Triatomic Molecules"
- 9:00 pm - 9:45 pm    **Joe Cline** (University of Nevada, USA)  
"Chiral Molecular Dynamics"
- 10:00 pm               Poster Session

**TUESDAY**

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Non-Adiabatic Dynamics and the Potential Energy Surface**Discussion Leader: **Laurie Butler** (University of Chicago, USA)9:00 am - 9:45 am **Millard Alexander** (University of Maryland, USA)"Electronic Adiabaticity in the F(Cl)+H<sub>2</sub> Abstraction Reactions"9:45 am - 10:30 am **Toshinori Suzuki** (Institute for Molecular Science, Japan)

"Non-Adiabatic Dynamics Probed by Charged Particle Imaging"

10:30 am Coffee Break

11:00 am - 11:45 am **David Yarkony** (Johns Hopkins University, USA)

"Conical intersections and the Spin-orbit Interaction: Beyond Diabolical"

11:45 am - 12:30 pm **Jingsong Zhang** (University of California Riverside, USA)

"Competitive Dissociation Pathways in Free Radical Photochemistry"

12:30 pm Lunch

1:30 pm - 6:00 pm Free Time

6:00 pm Dinner

7:30 pm - 9:45 pm **Inelastic Dynamics and the Potential Energy Surface**Discussion Leader: **Izhack Oref** (Technion-Israel Institute of Technology, Israel)7:30 pm - 8:15 pm **F. Javier Aoliz** (Universidad Complutense, Spain)

"Dynamics and Stereodynamics of Insertion Reactions"

8:30 pm - 9:30 pm **George Lendvay** (Hungarian Academy of Sciences, Hungary)

"Inelastic Scattering on Reactive Potential Surfaces"

9:00 pm - 9:45 pm **Amy Mullin** (Boston University, USA)

"New Tools for Predicting the Collisional Dynamics of High Energy Molecules"

10:00 pm Poster Session

**WEDNESDAY**

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Gas/Surface Dynamics and the Potential Energy Surface**Discussion Leader: **Bret Jackson** (University of Massachusetts, USA)9:00 am - 9:45 am **William Hase** (Wayne State University, USA)

"Energy Transfer and Chemical Reaction Dynamics in Gas/Surface Scattering. Rare Gas Atom to Peptide Projectiles"

9:45 am - 10:30 am **Geert-Jan Kroes** (Universiteit Leiden, The Netherlands)

"Vibrational effects on dissociative chemisorption of hydrogen: 6D quantum dynamics results for Cu(100) and Pt(111)"

10:30 am Coffee Break

11:00 am - 11:45 am **Alec Wodtke** (University of California at Santa Barbara, USA)

"Energy transfer of Stretched Molecules at Solid Surfaces"

11:45 am - 12:30 pm **Steven Sibener** (University of Chicago, USA)

"Scattering, Scanning Probe, and Numerical Simulation Studies of Dynamical Processes at Surfaces"

12:30 pm Lunch

1:30 pm - 6:00 pm Free Time

6:00 pm Dinner

7:30 pm - 9:30 pm **Clusters Involving Water and the Potential Energy Surface**Discussion Leader: **Karl Kleinermanns** (Universitat Dusseldorf, Germany)7:30 pm - 8:15 pm **Sotiris Xantheas** (Pacific Northwest National Laboratory, USA)

"Development of Solvent-Solute and Solute-Solute Interaction Models from First Principles: the Role of Clusters in Quantifying the Fundamental Interactions at the Molecular Level"

8:15 pm - 9:00 pm **Timothy Zwier** (Purdue University, USA)

"Laser probes of the potential energy landscapes and folding dynamics of small flexible

- biomolecules and their water-containing clusters"
- 8:30 pm - 9:45 pm **David Clary** (University College London, England)  
"Interaction of water with proteins"
- 10:00 pm Poster Session
- THURSDAY**
- 7:30 am - 8:30 am Breakfast
- 9:00 am - 12:30 pm **Clusters and the Potential Energy Surface**  
Discussion Leader: **Claude Leforestier** (Universite des Science et Techniques du Languedoc, France)
- 9:00 am - 9:45 am **Nadine Halberstadt** (Universite Paul Sabatier, France)  
"Energy Relaxation In van der Waals Clusters"
- 9:45 am - 10:30 am **Henning Meyer** (University of Georgia, USA)  
"Multiphoton spectroscopy of NO containing van der Waals complexes"
- 10:30 am Coffee Break
- 11:00 am - 11:45 am **Marsha Lester** (University of Pennsylvania, USA)  
"Exploring Reaction Coordinates Through Infrared Spectroscopy and Photo-Initiated Dynamics of OH Reactant Complexes"
- 11:45 am - 12:30 pm **K. Birgitta Whaley** (University of California at Berkeley, USA)  
"Molecular And Atomic Probes of Quantum Clusters - What Can We Learn and How Well Can We Know It?"
- 12:30 pm Lunch
- 1:30 pm - 6:00 pm Free Time
- 6:00 pm Dinner
- 7:30 pm **Three Body Interactions**  
Discussion Leader: **Albert Wagner** (Argonne National Laboratory, USA)
- 7:30 pm **Giacinto Scoles** (Princeton University, USA)  
"Chemistry, Physics and you: Three-body interactions are not easy"
- 10:00 pm Poster Session
- FRIDAY**
- 7:30 am - 8:30 am Breakfast
- 9:00 am Departure



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# ATOMIC & MOLECULAR INTERACTIONS

Roger Williams University  
Jul 7-12, 2002

**NOTE:** Receipt of Application does not guarantee acceptance to a Conference. Applications are reviewed by the Conference Chair. If the Chair approves your application, you become **Accepted** and you will be sent a personalized link to the GRC online registration site. When you complete the online registration, you become **Registered**.

Only those who have been **Accepted** or **Registered** will have their names listed below. Names of people who have only applied and have yet to be accepted will NOT appear.

Name	Organization	Participation	Status
MILLARD H ALEXANDER	UNIVERSITY OF MARYLAND	Speaker	Registered
STUART C ALTHORPE	UNIVERSITY OF DURHAM	Poster Presenter	Registered
FRANCISCO J AOIZ	UNIVERSIDAD COMPLUTENSE	Speaker	Registered
SULE ATAHAN	UNIVERSITY OF MARYLAND, CP	Poster Presenter	Registered
ANDREAS BACH	UNIVERSITY OF WISCONSIN - MADISON	Poster Presenter	Registered
ZLATKO BACIC	NEW YORK UNIVERSITY	Poster Presenter	Registered
JAMES W BARR	UNIVERSITY OF NEVADA, RENO	Poster Presenter	Registered
RAINER D BECK	EPFL	Poster Presenter	Registered
JOEL BOWMAN	EMORY UNIVERSITY	Speaker	Registered
LAURIE J BUTLER	THE UNIVERSITY OF CHICAGO	Speaker	Registered
DAVID C CLARY	UNIVERSITY COLLEGE LONDON	Speaker	Registered
JOSEPH I CLINE	UNIVERSITY OF NEVADA	Speaker	Registered
MICHAEL A COLLINS	AUSTRALIAN NATIONAL UNIVERSITY	Speaker	Registered
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YURI GEORGIEVSKI	SANDIA NATIONAL LABORATORIES	Poster Presenter	Registered
EVELYN M GOLDFIELD	WAYNE STATE UNIVERSITY	Speaker	Registered
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