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**GORDON RESEARCH CONFERENCES** *frontiers of science*

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**Nancy Ryan Gray, Ph.D.**  
Director

**2012 GORDON RESEARCH CONFERENCE & SEMINAR  
on ATOMIC & MOLECULAR INTERACTIONS**

**FINAL PROGRESS REPORT**

DEPARTMENT OF ENERGY  
GRANT NO. DE-SC0007766

The Gordon Research Conference on ATOMIC & MOLECULAR INTERACTIONS was held at Stonehill College Easton, Massachusetts, July 15-20, 2012. The Conference was well-attended with 121 participants (attendees list attached). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both U.S. and foreign scientists, senior researchers, young investigators, and students. Of the 121 attendees, 64 voluntarily responded to a general inquiry regarding ethnicity which appears on our registration forms. Of the 64 respondents, 11% were Minorities – 2% Hispanic, 9% Asian and 0% African American. Approximately 20% of the participants at the 2012 meeting were women.

The Gordon Research SEMINAR on ATOMIC & MOLECULAR INTERACTIONS was held at Stonehill College Easton, Massachusetts, July 14 - 15, 2012. The Conference was well-attended with 42 participants (attendees list attached). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both U.S. and foreign scientists, senior researchers, young investigators, and students. Of the 42 attendees, 20 voluntarily responded to a general inquiry regarding ethnicity which appears on our registration forms. Of the 20 respondents, 10% were Minorities – 0% Hispanic, 10% Asian and 0% African American. Approximately 29% of the participants at the 2012 meeting were women.

In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field.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. Attached is a copy of the formal schedule and speaker program and the poster program. 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.

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.

Sincerely,  
*Timothy S. Zwier, Conference Chairperson*  
PURDUE UNIVERSITY

Atomic & Molecular Interactions  
July 15-20, 2012  
Stonehill College  
Easton, MA  
Chair:  
**Timothy S. Zwier**

Vice Chair:  
**Sharon Hammes-Schiffer**

#### Related Meeting Information

The Atomic & Molecular Interactions Gordon Research Conference was held in conjunction with the **Atomic & Molecular Interactions Gordon Research Seminar**. Please refer to the Atomic & Molecular Interactions GRS web page for more information.

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The Atomic and Molecular Interactions Gordon Conference is justifiably recognized for its broad scope, touching on interactions occurring in isolated molecules, bimolecular collisions, clusters, aerosols, interfaces, and complex systems. The meeting has traditionally involved scientists engaged in fundamental research in gas and condensed phases and those who apply these concepts to systems of practical chemical and physical interest. A key tradition in this meeting is the strong mix of experiment and theory. The program for 2012 conference continues these traditions. At the 2012 AMI GRC, there will be talks in several broadly defined and partially overlapping areas:

- Intramolecular and single-collision reaction dynamics
- Photophysics and photochemistry of excited states
- Clusters, aerosols and solvation
- Interactions at interfaces
- Conformations and folding of large molecules
- Interactions under extreme conditions of temperature and pressure

These topics touch on a wide range of disciplines, grounded in physical chemistry, but reaching into biology, molecular physics, energy-related science, and astrochemistry, to name a few. The Conference will bring together a collection of investigators who are at the forefront of the field, and will provide opportunities for junior scientists and graduate students to present their work in poster format and exchange ideas with leaders in the field. Those wishing to present a poster should submit a brief abstract to the conference vice-chair. Some poster presenters will be selected for short talks. The collegial atmosphere of this Conference, with programmed discussion sessions as well as opportunities for informal gatherings in the afternoons and evenings, provides an avenue for scientists from different disciplines to brainstorm and promotes cross-disciplinary collaborations in the various research areas represented.

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#### Contributors



## SUNDAY

2:00 pm - 9:00 pm	Arrival and Check-in (Office Closed 6:00 pm - 7:00 pm)
6:00 pm	Dinner
7:30 pm - 7:35 pm	Welcome / Introductory Comments by GRC Site Staff
7:35 pm - 9:30 pm	<b>Single-collision and Intramolecular Dynamics I</b> Discussion Leader: <b>Timothy Zwier</b> (Purdue)
7:35 pm - 8:05 pm	<b>Arthur Suits</b> (Wayne State) "What don't we know and when didn't we know it: Are roaming reactions the Tectonic Plates of our field?"
8:05 pm - 8:15 pm	Discussion
8:15 pm - 8:45 pm	<b>Kopin Liu</b> (IAMS, Academia Sinica) "Controlling a chemical reaction by mode-, bond-excitations, and reactant alignment"
8:45 pm - 8:55 pm	Discussion
8:55 pm - 9:25 pm	<b>Laurie Butler</b> (Univ. Chicago) "Imaging and Scattering Studies of Radical Intermediates"
9:25 pm - 9:30 pm	Discussion
9:30 pm	Opening Reception

## MONDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>Clusters and Solvation</b> Discussion Leader: <b>David W. Pratt</b> (Univ. Pittsburgh)
9:00 am - 9:30 am	<b>Marsha Lester</b> (Univ. Pennsylvania) "Dynamical Outcomes of Quenching: Reflections on a Conical Intersection"

9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	<b>Joel Bowman</b> (Emory) "Full dimensional <i>ab initio</i> potentials and quantum vibrational dynamics of water clusters and hydrated ions"
10:10 am - 10:20 am	Discussion
10:20 am	Group Photo / Coffee Break
10:45 am - 11:15 am	<b>Gary Douberly</b> (Univ. Georgia) "Laser Spectroscopy of Metastable Open-Shell Clusters in Helium Nanodroplets"
11:15 am - 11:25 am	Discussion
11:25 am - 11:55 am	<b>Dor Ben-Amotz</b> (Purdue) "Vibrational spectroscopic detection of water structure changes in hydrophobic hydration shells"
11:55 am - 12:05 pm	Discussion
12:05 pm - 12:20 pm	Hot Topic Talk #1: <b>Amir Golan</b> (UC-Berkeley) "Post-ionization Relaxation in Hydrated Dimethyluracil"
12:20 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 6:00 pm	Free Time
6:00 pm	Dinner
7:30 pm - 9:30 pm	<b>Single-collision and intramolecular interactions II</b> Discussion Leader: <b>Takayuki Ebata</b> (Hiroshima Univ.)
7:30 pm - 8:00 pm	<b>Hanna Reisler</b> (Univ. Southern California) "Dynamical signatures of isomerization and dissociation in photoinitiated reactions of hydroxyalkyl radicals"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	<b>Martin Head-Gordon</b> (UC-Berkeley) "Energy decomposition analysis methods for intermolecular interactions: theory and applications"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	<b>Andrew Orr-Ewing</b> (Univ. Bristol, UK) "Chemical reaction dynamics from isolated collision to liquid solutions"
9:20 pm - 9:30 pm	Discussion
9:30 pm	<u>Poster Session I</u>

## TUESDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>Excited State interactions</b> Discussion Leader: <b>Wolfgang Domcke</b> (Technical Univ. Munich)
9:00 am - 9:30 am	<b>Samuel Leutwyler</b> (Univ. Berne)

	"Excitonic Interactions in Molecular Dimers: Experimental Splittings and Why Ab Initio Calculations Cannot Match Them"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	<b>Spiridoula Matsika</b> (Temple Univ.) "Non-adiabatic events in interacting chromophores"
10:10 am - 10:20 am	Discussion
10:20 am	Coffee Break
10:45 am - 11:15 am	<b>Anne Zehnacker-Rentien</b> (Université Paris XI) "Stereochemistry effects in the gas-phase photophysics of quinine derivatives"
11:15 am - 11:25 am	Discussion
11:25 am - 11:55 am	<b>Todd Martinez</b> (Stanford) "New Perspectives in Excited state dynamics"
11:55 am - 12:05 pm	Discussion
12:05 pm - 12:20 pm	Hot Topic Talk #2: <b>Nadia Doslic</b> (Boskovic Institute, Croatia) "Mechanisms of Non-radiative Deactivation in Model Peptides"
12:20 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 6:00 pm	Free Time
6:00 pm	Dinner
7:30 pm - 9:30 pm	<b>Charges and excited states in solution and on ice</b> Discussion Leader: <b>Sharon Hammes-Schiffer</b> (Penn State)
7:30 pm - 8:00 pm	<b>David McCamant</b> (Univ. Rochester) "Ultrafast condensed phase photochemistry probed with femtosecond stimulated Raman spectroscopy"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	<b>David VandenBout</b> (Univ. of Texas-Austin) "Single molecule spectroscopy of chain-chain interactions in conjugated polymers"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	<b>Bruce Kay</b> (PNNL) "Beakers without walls: Using nanoscale amorphous solid films to create and study deeply supercooled liquids"
9:20 pm - 9:30 pm	Discussion
9:30 pm	<u>Poster Session II</u>

## WEDNESDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>Interactions at Interfaces, Surfaces, and Aerosols</b> Discussion Leader: <b>David Nesbitt</b> (JILA)

9:00 am - 9:30 am	<b>Alec Wodtke</b> (Univ. Gottingen) "Chemical Dynamics at Surfaces"
9:30 am - 9:40 am	Discussion
9:40 am - 10:10 am	<b>Ruth Signorell</b> (Univ. British Columbia) "Characterization of Clusters and Ultrafine Aerosols by Ultraviolet Photoionization"
10:10 am - 10:20 am	Discussion
10:20 am	Coffee Break
10:45 am - 11:15 am	<b>John Tully</b> (Yale) "Excited State Dynamics at Surfaces"
11:15 am - 11:25 am	Discussion
11:25 am - 11:55 am	<b>Gil Nathanson</b> (Univ. Wisconsin-Madison) "Non-Maxwellian Evaporation of Helium from Liquid Hydrocarbons, Ethylene Glycol, and Water"
11:55 am - 12:05 pm	Discussion
12:05 pm - 12:20 pm	Hot Topic Talk #3: <b>Joseph Subotnik</b> (Penn) "Multiple, Consecutive Scattering Events and Curve-Crossings"
12:20 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 6:00 pm	Free Time
6:00 pm	Dinner
7:00 pm - 7:30 pm	<u>Business Meeting</u> <i>Nominations for the next Vice Chair; Fill out Conference Evaluation Forms; Discuss future Site &amp; Scheduling preferences; Election of the next Vice Chair</i>
7:30 pm - 9:30 pm	<b>Conformations and Folding</b> Discussion Leader: <b>Philippe Dugourd</b> (Univ. Lyon, France)
7:30 pm - 8:00 pm	<b>Tom Rizzo</b> (EPFL) "Metastable conformations of electrosprayed peptides revealed by IR and UV spectroscopy"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:40 pm	<b>William Noid</b> (Penn State) "Specific and nonspecific effects of glycosylation upon a disordered peptide"
8:40 pm - 8:50 pm	Discussion
8:50 pm - 9:20 pm	<b>Ashok Deniz</b> (Scripps Research Institute) "Single-Molecule Dynamics and Binding-Coupled Folding of Intrinsically Disordered Proteins"
9:20 pm - 9:30 pm	Discussion
9:30 pm	<u>Poster Session III</u>

## THURSDAY

7:30 am - 8:30 am Breakfast

### 9:00 am - 12:30 pm **Interactions under Extreme Conditions**

Discussion Leader: **Stephen Klippenstein** (Argonne)

9:00 am - 9:30 am **Gerard Meijer** (Fritz Haber Institute, Germany)  
"Taming Molecular Beams"

9:30 am - 9:40 am Discussion

9:40 am - 10:10 am **Ian R. Sims** (Univ. Rennes)  
"Experimental investigations of radical-molecule reactions using low temperature supersonic flows"

10:10 am - 10:20 am Discussion

10:20 am Coffee Break

10:45 am - 11:15 am **Craig Taatjes** (Combustion Research Facility)  
"Fundamental Autoignition Chemistry at High Pressure"

11:15 am - 11:25 am Discussion

11:25 am - 11:55 am **Tim Strobel** (Carnegie Institute)  
"Intermolecular Interactions at Extreme Pressures"

11:55 am - 12:05 pm Discussion

12:05 pm - 12:20 pm Hot Topic Talk #4: **Vasilios Stavros** (Warwick, UK)  
"Pre-biotic earth: Comparing the ultraviolet photostability of azole chromophores"

12:20 pm - 12:30 pm Discussion

12:30 pm Lunch

1:30 pm - 6:00 pm Free Time

6:00 pm Dinner

### 7:30 pm - 9:30 pm **Longer (range), shorter (timescales), stronger (fields), weaker (interactions)**

Discussion Leader: **Martin Quack** (ETH-Zurich)

7:30 pm - 8:00 pm **Ken Jordan** (Univ. Pittsburgh)  
"On the Role of Long-range Interactions in (H<sub>2</sub>O)<sub>n</sub>- Clusters: From Many-body Theory to Model Potentials"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:40 pm **Steve Leone** (UC-Berkeley)  
"X-ray investigations of electron dynamics toward the attosecond limit"

8:40 pm - 8:50 pm Discussion

8:50 pm - 9:20 pm **Tim Softley** (Oxford)  
"Sub-Kelvin chemistry using laser-cooled ions"

9:20 pm - 9:30 pm Discussion

**FRIDAY**

7:30 am - 8:30 am      Breakfast

9:00 am                      Departure

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Atomic & Molecular Interactions  
Gordon Research Seminar  
July 14-15, 2012  
Stonehill College  
Easton, MA  
Chair:  
**Amanda S. Case**

Associate Chair:  
**Julia H. Lehman**

#### Related Meeting Information

The Atomic & Molecular Interactions Gordon Research Seminar was held in conjunction with the **Atomic & Molecular Interactions Gordon Research Conference**. Please refer to the Atomic & Molecular Interactions GRC web page for more information.

The Gordon Research Seminar on Atomic & Molecular Interactions is a unique forum for graduate students, post-docs, and other scientists with comparable levels of experience and education to present and exchange new data and cutting edge ideas.

The theme of this meeting, in keeping with the tradition of the Atomic and Molecular Interactions Gordon Research Conference, is far-reaching and involves fundamental research in the gas and condensed phases along with application of these ideas to practical chemical fields. The oral presentations, which will contain a combination of both experiment and theory, will focus on four broad categories:

- Ultrafast Phenomena
- Excited States, Photoelectrons, and Photoions
- Chemical Reaction Dynamics
- Biomolecules and Clusters

#### Contributors



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## SATURDAY

1:00 pm - 5:00 pm	Arrival and Check-in
3:30 pm - 3:50 pm	Introductory Comments by GRC Site Staff / Welcome by the GRS Conference Chair
3:50 pm - 4:30 pm	<b>Ultrafast Phenomena</b>
3:50 pm - 4:05 pm	<b>Fawzi Abou-Chahine</b> (University of Bristol) "Chemical Reaction and Vibrational Relaxation in Solution: The HCl Story"
4:05 pm - 4:10 pm	Discussion
4:10 pm - 4:25 pm	<b>Jeremy Viau Trudel</b> (Laval University) "Molecular Ionization by an Intense Attosecond XUV Pulse: Is a Franck-Condon Approximation Acceptable?"
4:25 pm - 4:30 pm	Discussion
4:30 pm - 6:00 pm	<u>Poster Session I</u>
6:00 pm	Dinner
7:30 pm - 9:30 pm	<b>Biomolecules and Clusters</b>
	Discussion Leader: <b>Ruth Signorell</b> (University of British Columbia)
7:30 pm - 8:00 pm	Keynote Speaker: <b>Kenneth Jordan</b> (University of Pittsburgh) "Accommodation of Excess Electrons and Protons by Water Clusters"
8:00 pm - 8:10 pm	Discussion
8:10 pm - 8:25 pm	<b>Andrew Deblase</b> (Yale University) "Characterization of Charged Intramolecular Hydrogen Bonds in Protonated Proton Sponges by Vibrational Predissociation Spectroscopy"
8:25 pm - 8:30 pm	Discussion
8:30 pm - 8:45 pm	<b>Philipp Marquetand</b> (University of Vienna) "The Role of Intersystem Crossing in the Photorelaxation of the DNA Nucleobase Cytosine: a Surface Hopping Study"
8:45 pm - 8:50 pm	Discussion
8:50 pm - 9:05 pm	<b>Jacob Dean</b> (Purdue University) "Mixed Helices in the Gas Phase: Conformation-specific UV and IR Spectroscopy of Polyglycine Z-(Gly) <sub>n</sub> (n=1,3,5)"
9:05 pm - 9:10 pm	Discussion
9:10 pm - 9:25 pm	<b>Dominik Pentlehner</b> (University of Aarhus) "Laser Induced Alignment of Molecules in Helium Droplets"
9:25 pm - 9:30 pm	Discussion

## SUNDAY

7:30 am - 8:30 am	Breakfast
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9:00 am - 11:00 am	<b>Excited States, Photoelectrons, and Photoions</b>
	Discussion Leader: <b>Julia Lehman</b> (University of Pennsylvania)
9:00 am - 9:40 am	<u>Panel Discussion:</u> "Making Yourself Standout as a Scientist" <b>Kenneth Jordan</b> (University of Pittsburgh), <b>Andrew Orr-Ewing</b> (University of Bristol), <b>Ruth Signorell</b> (University of British Columbia), and <b>Timothy Zwier</b> (Purdue University)
9:40 am - 9:55 am	<b>Andrew Petit</b> (Ohio State University) "Exploring the Effects of Rotation-vibration Coupling in Highly Fluxional Molecules Using Diffusion Monte Carlo"
9:55 am - 10:00 am	Discussion
10:00 am - 10:15 am	<b>Joseph Beames</b> (University of Pennsylvania) "A New Spectroscopic Window on Hydroxyl Radicals Using UV+VUV Resonant Ionization"
10:15 am - 10:20 am	Discussion
10:20 am - 10:35 am	<b>Bernadette Broderick</b> (Wayne State University) "The Dynamic Stark Effect and Ozone: Control Over Electronic State Branching"
10:35 am - 10:40 am	Discussion
10:40 am - 10:55 am	<b>Lori Culberson</b> (University of Arizona) "Electronic Structure and Relative Stability of Heterocyclic Radicals via Anion Photoelectron Imaging"
10:55 am - 11:00 am	Discussion
11:00 am - 12:30 pm	<u>Poster Session II</u> <i>Coffee will be served in the poster area from 11:00 am - 11:30 am</i>
12:30 pm	Lunch
1:30 pm - 2:30 pm	<b>Chemical Reactions Dynamics</b>
	Discussion Leader: <b>Andrew Orr-Ewing</b> (University of Bristol)
1:30 pm - 1:45 pm	<b>Monika Gruetter</b> (JILA, CU Boulder) "Quantum State-resolved Reactive and Inelastic Scattering at Gas-liquid and Gas-solid Interfaces"
1:45 pm - 1:50 pm	Discussion
1:50 pm - 2:05 pm	<b>Amit Kumar Samanta</b> (University of Southern California) "Imaging the Vibrational Predissociation of Water Dimers"
2:05 pm - 2:10 pm	Discussion
2:10 pm - 2:25 pm	<b>Amit Sharma</b> (Argonne National Lab) "The Role of Radical-complex Intermediates in High-pressure Chemistry"
2:25 pm - 2:30 pm	Discussion
2:30 pm - 3:00 pm	<u>Evaluation Period</u> <i>Fill out GRS Evaluation Forms</i>

3:00 pm

Gordon Research Seminar ends. For those attending the associated Gordon Research Conference, please check in at the GRC Office beginning at 4:00 pm.

**Atomic & Molecular Interactions (2012)**

<b>Name</b>	<b>Organization</b>	<b>Participation</b>	<b>Status</b>
<b>ABEYSEKERA, CHAMARA S</b>	WAYNE STATE UNIVERSITY	Poster Presenter	Registered
<b>ABOU-CHAHINE, FAWZI</b>	UNIVERSITY OF BRISTOL	Poster Presenter	Registered
<b>BEAMES, JOSEPH M</b>	UNIVERSITY OF PENNSYLVANIA	Poster Presenter	Registered
<b>BEDRANE, ZEYNEB</b>	TLEMCEN UNIVERSITY	Poster Presenter	Registered
<b>BEN-AMOTZ, DOR</b>	PURDUE UNIVERSITY	Speaker	Registered
<b>BERRIOS, EDUARDO</b>	UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN	Poster Presenter	Registered
<b>BOWMAN, JOEL</b>	EMORY UNIVERSITY	Speaker	Registered
<b>BRODERICK, BERNADETTE M</b>	WAYNE STATE UNIVERSITY	Attendee	Registered
<b>BUCHANAN, EVAN G</b>	PURDUE UNIVERSITY	Poster Presenter	Registered
<b>BUTLER, LAURIE J</b>	UNIVERSITY OF CHICAGO	Speaker	Registered
<b>CASE, AMANDA S</b>	UNIVERSITY OF COLORADO	Poster Presenter	Registered
<b>CHOI, JONG-HO</b>	KOREA UNIVERSITY	Poster Presenter	Registered
<b>COLE-FILIPAK, NEIL C</b>	UNIVERSITY OF CALIFORNIA, BERKELEY	Poster Presenter	Registered
<b>COOPER, RUSSELL</b>	AFRL	Poster Presenter	Registered
<b>CULBERSON, LORI</b>	UNIVERSITY OF ARIZONA	Poster Presenter	Registered
<b>DEAN, JACOB C</b>	PURDUE UNIVERSITY	Poster Presenter	Registered
<b>DEBLASE, ANDREW F</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>DENIZ, ASHOK</b>	SCRIPPS RESEARCH INSTITUTE	Speaker	Registered
<b>DILLON, JOSEPH J</b>	JOHNS HOPKINS UNIVERSITY	Poster Presenter	Registered
<b>DOMCKE, WOLFGANG</b>	TECHNICAL UNIVERSITY MUNICH	Discussion Leader	Registered
<b>DOSLIC, NADJA</b>	RUDJER BOSKOVIC INSTITUTE	Poster Presenter	Registered
<b>DOUBERLY, GARY</b>	UNIVERSITY OF GEORGIA	Speaker	Registered
<b>DOYLE, MICHAEL B</b>	WAYNE STATE UNIVERSITY	Poster Presenter	Registered
<b>DUCHOVIC, RONALD J</b>	INDIANA UNIVERSITY PURDUE UNIVERSITY FORT WAYNE	Poster Presenter	Registered
<b>DUGOURD, PHILIPPE</b>	UNIVERSITY OF LYON - CNRS	Discussion Leader	Registered
<b>EBATA, TAKAYUKI</b>	HIROSHIMA UNIVERSITY	Discussion Leader	Registered
<b>FANG, YIGANG</b>	QUEENS COLLEGE, CUNY	Poster Presenter	Registered
<b>FLEISHER, ADAM J</b>	JILA, UNIVERSITY OF COLORADO	Poster Presenter	Registered
<b>GAO, HONG</b>	UCDAVIS	Poster Presenter	Registered
<b>GOLAN, AMIR</b>	LAWRENCE BERKELEY NATIONAL LAB	Poster Presenter	Registered
<b>GOLDBERG, NOAH T</b>	AGILENT LABORATORIES	Poster Presenter	Registered
<b>GORDON, ROBERT J</b>	UNIVERSITY OF ILLINOIS AT CHICAGO	Poster Presenter	Registered
<b>GRUETTER, MONIKA</b>	JILA, UNIVERSITY OF COLORADO AT BOULDER	Poster Presenter	Registered
<b>GUNAWARDENA, MEVAN</b>	STONEHILL COLLEGE	Poster Presenter	Registered
<b>HAMMES-SCHIFFER, SHARON</b>	UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN	Vice Chair	Registered
<b>HAPKA, MICHAL J.</b>	UNIVERSITY OF WARSAW	Poster Presenter	Registered
<b>HAUSE, MICHAEL L</b>	AIR FORCE RESEARCH LABORATORY	Poster Presenter	Registered
<b>HEAD-GORDON, MARTIN</b>	UNIVERSITY OF CALIFORNIA, BERKELEY	Speaker	Registered

<b>HEID, CORNELIA G.</b>	UNIVERSITY OF WISCONSIN-MADISON	Poster Presenter	Registered
<b>HOMAYOON, ZAHRA</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>JACOBSON, LEIF D</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>JIA, BEIKE</b>	GORDON COLLEGE	Attendee	Registered
<b>JOALLAND, BAPTISTE</b>	WAYNE STATE UNIVERSITY	Poster Presenter	Registered
<b>JOBINS, MATTHEW M</b>	UNIVERSITY OF NOTRE DAME	Poster Presenter	Registered
<b>JOHNSON, CHRISTOPHER J</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>JORDAN, KENNETH D</b>	UNIVERSITY OF PITTSBURGH	Speaker	Registered
<b>KAY, BRUCE D</b>	PACIFIC NORTHWEST NATIONAL LABORATORY	Speaker	Registered
<b>KLIPPENSTEIN, STEPHEN</b>	ARGONNE NATIONAL LABORATORIES	Discussion Leader	Registered
<b>KOEHLER, SVEN P K</b>	UNIVERSITY OF MANCHESTER	Poster Presenter	Registered
<b>KOH, CHRISTINE J</b>	UNIVERSITY OF CALIFORNIA, BERKELEY	Poster Presenter	Registered
<b>KOPLITZ, BRENT D</b>	TULANE UNIVERSITY	Attendee	Registered
<b>KUMAR, AJITESH</b>	IIT KANPUR INDIA	Poster Presenter	Registered
<b>LAM, CHOW-SHING</b>	JAMES FRANCK INSTITUTE, UNIVERSITY OF CHICAGO	Poster Presenter	Registered
<b>LAYFIELD, JOSHUA P</b>	PENN STATE UNIVERSITY	Poster Presenter	Registered
<b>LEAVITT, CHRISTOPHER</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>LEHMAN, JULIA H</b>	UNIVERSITY OF PENNSYLVANIA	Poster Presenter	Registered
<b>LEONE, STEPHEN</b>	UNIVERSITY OF CALIFORNIA, BERKELEY	Speaker	Registered
<b>LESTER, MARSHA I</b>	UNIVERSITY OF PENNSYLVANIA	Speaker	Registered
<b>LEUTWYLER, SAMUEL</b>	UNIVERSITY OF BERN	Speaker	Registered
<b>LITMAN, JESSICA H</b>	UNIVERSITY OF BRITISH COLUMBIA	Poster Presenter	Registered
<b>LIU , KOPIN</b>	INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES (IAMS)	Speaker	Registered
<b>LIU, HANCHAO</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>LOCKYEAR, JESSICA F</b>	LAWRENCE BERKELEY NATIONAL LABORATORY	Poster Presenter	Registered
<b>LU, ZHEN</b>	TEMPLE UNIVERSITY	Poster Presenter	Registered
<b>LUCAS, BRUNO</b>	CNRS	Poster Presenter	Registered
<b>MA, QIANLI</b>	JOHNS HOPKINS UNIVERSITY	Poster Presenter	Registered
<b>MARQUETAND, PHILIPP</b>	UNIVERSITY OF VIENNA	Poster Presenter	Registered
<b>MARTINEZ, TODD J</b>	STANFORD UNIVERSITY	Speaker	Registered
<b>MATSIKA, SPIRIDOULA</b>	TEMPLE UNIVERSITY	Speaker	Registered
<b>MATSUMOTO, YOSHITERU</b>	UNIVERSITY OF HYOGO	Poster Presenter	Registered
<b>MCBANE, GEORGE C</b>	GRAND VALLEY STATE UNIVERSITY	Poster Presenter	Registered
<b>MCCAMANT, DAVID W</b>	UNIVERSITY OF ROCHESTER	Speaker	Registered
<b>MCGLYNN, SHANE J</b>	TUALNE	Poster Presenter	Registered
<b>MCGURK, STEPHEN J</b>	HERIOT-WATT UNIVERSITY	Poster Presenter	Registered
<b>MEIJER, GERARD</b>	FRITZ-HABER-INSTITUT DER MAX-PLANCK-GESELLSCHAFT	Speaker	Registered
<b>MIYABE, SHUNGO</b>	STANFORD UNIVERSITY	Poster Presenter	Registered
<b>NATHANSON, GILBERT M</b>	UNIVERSITY OF WISCONSIN-MADISON	Speaker	Registered
<b>NEGRU, BOGDAN</b>	UNIVERSITY OF CALIFORNIA BERKELEY	Poster Presenter	Registered
<b>NESBITT, DAVID J</b>	UNIVERSITY OF COLORADO AT BOULDER	Discussion	Registered

		Leader	
<b>NOID, WILLIAM G</b>	PENNSYLVANIA STATE UNIVERSITY	Speaker	Registered
<b>OLDHAM, JAMES M</b>	WAYNE STATE UNIVERSITY	Poster Presenter	Registered
<b>ORR-EWING, ANDREW</b>	UNIVERSITY OF BRISTOL	Speaker	Registered
<b>PENTLEHNER, DOMINIK</b>	UNIVERSITY OF AARHUS	Poster Presenter	Registered
<b>PETERS, MICHEL</b>	UNIVERSITY LAVAL	Poster Presenter	Registered
<b>PETIT, ANDREW S</b>	OHIO STATE UNIVERSITY	Poster Presenter	Registered
<b>PETROVIC, VLADIMIR S</b>	STANFORD UNIVERSITY	Poster Presenter	Registered
<b>PRATT, DAVID</b>	UNIVERSITY OF VERMONT	Discussion Leader	Registered
<b>QU, CHEN</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>QUACK, MARTIN</b>	ETH ZURICH	Discussion Leader	Registered
<b>REISLER, HANNA</b>	UNIVERSITY OF SOUTHERN CALIFORNIA	Speaker	Registered
<b>RIZZO, THOMAS R</b>	ECOLE POLYTECHNIQUE FEDERALE LAUSANNE	Speaker	Registered
<b>ROBERTS, GARETH M</b>	UNIVERSITY OF WARWICK	Poster Presenter	Registered
<b>ROY, SHARANI</b>	NORTHWESTERN UNIVERSITY	Poster Presenter	Registered
<b>SAMANTA, AMIT KUMAR</b>	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
<b>SCHNITZER, CHERYL S</b>	STONEHILL COLLEGE	Poster Presenter	Registered
<b>SCHUURMAN, MICHAEL S</b>	NATIONAL RESEARCH COUNCIL OF CANADA	Poster Presenter	Registered
<b>SHARMA, AMIT R</b>	ARGONNE NATIONAL LAB	Poster Presenter	Registered
<b>SIGNORELL, RUTH</b>	UNIVERSITY OF BRITISH COLUMBIA	Speaker	Registered
<b>SIMS, IAN R</b>	UNIVERSITE DE RENNES 1	Speaker	Registered
<b>SMITH, DANIEL G</b>	AUBURN UNIVERISTY	Poster Presenter	Registered
<b>SOFTLEY, TIMOTHY P</b>	UNIVERSITY OF OXFORD	Speaker	Registered
<b>SRIVASTAVA, RAJESH R</b>	INDIAN INSTITUTE OF TECHNOLOGY ROORKEE	Poster Presenter	Registered
<b>SRIVASTAVA, SAURABH</b>	INDIAN INSTITUTE OF TECHNOLOGY KANPUR	Poster Presenter	Registered
<b>STAVROS, VASILIOS G</b>	UNIVERSITY OF WARWICK	Poster Presenter	Registered
<b>STEARNS, JAIME A</b>	AIR FORCE RESEARCH LAB	Attendee	Registered
<b>STROBEL, TIMOTHY</b>	CARNEGIE INSTITUTION OF WASHINGTON	Speaker	Registered
<b>SUBOTNIK, JOSEPH E</b>	UNIVERSITY OF PENNSYLVANIA	Attendee	Registered
<b>SUITS, ARTHUR G</b>	WAYNE STATE UNIVERSITY	Speaker	Registered
<b>TAATJES, CRAIG</b>	SANDIA NATIONAL LABORATORY	Speaker	Registered
<b>TIWARI, VIVEK</b>	UNIVERSITY OF COLORADO, BOULDER	Poster Presenter	Registered
<b>TULLY, JOHN C</b>	YALE UNIVERSITY	Speaker	Registered
<b>VANDEN BOUT, DAVID A</b>	UNIVERSITY OF TEXAS AT AUSTIN	Speaker	Registered
<b>VIAU TRUDEL, JEREMY</b>	LAVAL UNIVERSITY	Poster Presenter	Registered
<b>WANG, XIAOHONG</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>WEST, ADAM H C</b>	SIGNORELL GROUP	Poster Presenter	Registered
<b>WODTKE, ALEC</b>	MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY	Speaker	Registered
<b>YAN, LU</b>	WAYNE STATE UNIVERSITY	Poster Presenter	Registered
<b>ZEHNACKER-RENTIEN, ANNE</b>	CNRS UNIVERSITY PARIS SUD	Speaker	Registered
<b>ZHELDAKOV, IGOR L.</b>	UNIVERSITY OF KANSAS	Poster Presenter	Registered
<b>ZHU, XIAOLEI</b>	JOHNS HOPKINS UNIVERSITY	Poster Presenter	Registered

**ZWIER, TIMOTHY S**  
**121 Attendees**

PURDUE UNIVERSITY

Chair

Registered



**Atomic & Molecular Interactions (GRS) (2012)**

<b>Name</b>	<b>Organization</b>	<b>Participation</b>	<b>Status</b>
<b>ABOU-CHAHINE, FAWZI</b>	UNIVERSITY OF BRISTOL	Speaker	Registered
<b>BEAMES, JOSEPH M</b>	UNIVERSITY OF PENNSYLVANIA	Speaker	Registered
<b>BEDRANE, ZEYNEB</b>	TLEMCEN UNIVERSITY	Poster Presenter	Registered
<b>BRODERICK, BERNADETTE M</b>	WAYNE STATE UNIVERSITY	Speaker	Registered
<b>BUCHANAN, EVAN G</b>	PURDUE UNIVERSITY	Poster Presenter	Registered
<b>CASE, AMANDA S</b>	UNIVERSITY OF COLORADO	Chair	Registered
<b>COOPER, RUSSELL</b>	AFRL	Poster Presenter	Registered
<b>CULBERSON, LORI</b>	UNIVERSITY OF ARIZONA	Speaker	Registered
<b>DEAN, JACOB C</b>	PURDUE UNIVERSITY	Speaker	Registered
<b>DEBLASE, ANDREW F</b>	YALE UNIVERSITY	Speaker	Registered
<b>FANG, YIGANG</b>	QUEENS COLLEGE, CUNY	Poster Presenter	Registered
<b>FLEISHER, ADAM J</b>	JILA, UNIVERSITY OF COLORADO	Poster Presenter	Registered
<b>GRUETTER, MONIKA</b>	JILA, UNIVERSITY OF COLORADO AT BOULDER	Speaker	Registered
<b>HAPKA, MICHAL J.</b>	UNIVERSITY OF WARSAW	Poster Presenter	Registered
<b>HEID, CORNELIA G.</b>	UNIVERSITY OF WISCONSIN-MADISON	Poster Presenter	Registered
<b>JACOBSON, LEIF D</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>JOBBINS, MATTHEW M</b>	UNIVERSITY OF NOTRE DAME	Poster Presenter	Registered
<b>JOHNSON, CHRISTOPHER J</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>JORDAN, KENNETH D</b>	UNIVERSITY OF PITTSBURGH	Speaker	Registered
<b>LAYFIELD, JOSHUA P</b>	PENN STATE UNIVERSITY	Poster Presenter	Registered
<b>LEAVITT, CHRISTOPHER</b>	YALE UNIVERSITY	Poster Presenter	Registered
<b>LEHMAN, JULIA H</b>	UNIVERSITY OF PENNSYLVANIA	Chair	Registered
<b>LI, WEILI</b>	BROWN UNIVERSITY	Poster Presenter	Registered
<b>LITMAN, JESSICA H</b>	UNIVERSITY OF BRITISH COLUMBIA	Poster Presenter	Registered
<b>LIU, HANCHAO</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>LU, ZHEN</b>	TEMPLE UNIVERSITY	Poster Presenter	Registered
<b>MARQUETAND, PHILIPP</b>	UNIVERSITY OF VIENNA	Speaker	Registered
<b>MCGLYNN, SHANE J</b>	TUALNE	Poster Presenter	Registered
<b>MCGURK, STEPHEN J</b>	HERIOT-WATT UNIVERSITY	Poster Presenter	Registered
<b>MIYABE, SHUNGO</b>	STANFORD UNIVERSITY	Poster Presenter	Registered
<b>ORR-EWING, ANDREW</b>	UNIVERSITY OF BRISTOL	Discussion Leader	Registered
<b>PENTLEHNER, DOMINIK</b>	UNIVERSITY OF AARHUS	Speaker	Registered
<b>PETERS, MICHEL</b>	UNIVERSITY LAVAL	Poster Presenter	Registered
<b>PETIT, ANDREW S</b>	OHIO STATE UNIVERSITY	Speaker	Registered
<b>QU, CHEN</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>ROY, SHARANI</b>	NORTHWESTERN UNIVERSITY	Poster Presenter	Registered
<b>SAMANTA, AMIT KUMAR</b>	UNIVERSITY OF SOUTHERN CALIFORNIA	Speaker	Registered
<b>SIGNORELL, RUTH</b>	UNIVERSITY OF BRITISH COLUMBIA	Discussion Leader	Registered
<b>VIAU TRUDEL, JEREMY</b>	LAVAL UNIVERSITY	Speaker	Registered
<b>WANG, XIAOHONG</b>	EMORY UNIVERSITY	Poster Presenter	Registered
<b>WEST, ADAM H C</b>	SIGNORELL GROUP	Poster Presenter	Registered
<b>ZWIER, TIMOTHY S</b>	PURDUE UNIVERSITY	Poster Presenter	Registered

**42 Attendees**