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

**2006 GORDON RESEARCH CONFERENCE  
on MOLECULAR & IONIC CLUSTERS  
FINAL PROGRESS REPORT**

DEPARTMENT OF ENERGY  
GRANT NO. DE-FG02-05ER15737

The Gordon Research Conference (GRC) on MOLECULAR & IONIC CLUSTERS was held at Crowne Plaza from 2/19/2006 thru 2/24/2006. The Conference was well-attended with 89 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.

In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field.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.

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 As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings.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.

Sincerely,

**MICHAEL A DUNCAN**  
UNIVERSITY OF GEORGIA

# Molecular & Ionic Clusters

February 19-24, 2006  
Crowne Plaza  
Ventura, CA

Chairs: **Michael A Duncan** & **Sotiris S Xantheas**  
Vice Chairs: **Jeremy M Hutson** & **Dan Neumark**

## SUNDAY

4:00 pm - 9:00 pm	Arrival and Check-in
6:00 pm	Dinner
7:30 pm - 9:30 pm	<b>ASTROPHYSICAL CLUSTERS</b>
7:30 pm - 7:45 pm	Overview by Discussion Leader: <b>Bill Klemperer</b> (Harvard Univ., USA) "Interstellar Chemistry; Why so many unsaturated carbon chains and can weakly bound complexes occur?"
7:45 pm - 8:30 pm	<b>Michael McCarthy</b> (Harvard Univ., USA) "Small Carbon, Silicon, and Sulfur Clusters in the Laboratory and in Space"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	<b>John Maier</b> (Univ. of Basel, Switzerland) "Gas Phase Electronic Spectra of Carbon-Containing Molecules of Relevance to Astrophysics"
9:20 pm - 9:30 pm	Discussion

## MONDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>REACTIONS AND RADICALS</b>
9:00 am - 9:15 am	Overview by Discussion Leader: <b>Dan Neumark</b> (UC-Berkeley, USA) "Photoinduced reactions in clusters"
9:15 am - 10:00 am	<b>Marsha Lester</b> (Univ. of Pennsylvania, USA) "Intermolecular Interactions and Reactions of Hydroxyl Radicals: A New View"
10:00 am - 10:10 am	Discussion
10:10 am	Conference Photo / Coffee Break
10:40 am - 11:25 am	<b>Joe Francisco</b> (Purdue Univ., USA) "New Perspectives on Radical Reactions in Atmospheric Chemical Processes"
11:25 am - 11:35 am	Discussion
11:35 am - 12:20 pm	<b>Anna Krylov</b> (USC, USA) "Complex photodissociation of weakly bound covalent NO dimer: Insights from electronic structure calculations"
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>HELIUM DROPLETS</b>
7:30 pm - 7:45 pm	Overview by Discussion Leader: <b>Andrey Vilessov</b> (Univ. of Southern California, USA) "Molecules, superfluidity and He droplets"

7:45 pm - 8:30 pm	<b>Birgitta Whaley</b> (UC-Berkeley, USA) "Spectroscopy and Superfluidity in Helium Droplets"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	<b>Martina Havenith</b> (Ruhr Univ. Bochum, Germany) "Probing phonon-rotational coupling: IR spectroscopy of dopants in helium nanodroplets"
9:20 pm - 9:30 pm	Discussion
9:45 pm -	Poster Session 1

## TUESDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>METAL CLUSTERS AND COMPLEXES</b>
9:00 am - 9:15 am	Overview by Discussion Leader: <b>Will Castleman</b> (Penn State Univ., USA) "Exploring Metal Clusters"
9:15 am - 10:00 am	<b>Martin Jarrold</b> (Indiana Univ., USA) "Cluster Melting"
10:00 am - 10:10 am	Discussion
10:10 am	Coffee Break
10:40 am - 11:25 am	<b>Atsushi Nakajima</b> (Keio Univ., Japan) "Electronic and Geometric Properties of Metal Encapsulated or Sandwiched Clusters"
11:25 am - 11:35 am	Discussion
11:35 am - 12:20 pm	<b>Kit Bowen</b> (Johns-Hopkins Univ., USA) "Photoelectron Spectroscopy of Cluster Anions"
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>IONIC CLUSTERS</b>
7:30 pm - 7:45 pm	Overview by Discussion Leader: <b>Jim Lisz</b> (Univ. of Illinois, USA) "Recent Developments in Ionic Clusters"
7:45 pm - 8:30 pm	<b>Masaaki Fuji</b> (Univ. of Tokyo, Japan) "Real-time observation of ionization induced site switching in aromatic clusters"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	<b>Lai-Sheng Wang</b> (Pacific Northwest National Lab, USA) "Probing the Electronic, Structural, and Chemical Properties of Metal Clusters Using Anion Photoelectron Spectroscopy"
9:20 pm - 9:30 pm	Discussion
9:45 pm -	Poster Session 2

## WEDNESDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>HYDROGEN-BONDED NETWORKS</b>
9:00 am - 9:15 am	Overview by Discussion Leader: <b>Ken Jordan</b> (Univ. of Pittsburgh, USA) "Overview of Hydrogen-Bonded Systems"
9:15 am - 10:00 am	<b>Mark Johnson</b> (Yale Univ., USA) "Water Clusters: A Bottom-up Approach to Aqueous Chemistry"
10:00 am - 10:10 am	Discussion

10:10 am	Coffee Break
10:40 am - 11:25 am	<b>Anne McCoy</b> (Ohio State Univ., USA) "Investigations of the Dynamics and Spectroscopy of $\text{H}_3\text{O}_2^-$ and $\text{H}_5\text{O}_2^+$ using Quantum Monte Carlo"
11:25 am - 11:35 am	Discussion
11:35 am - 12:20 pm	<b>Martin Suhm</b> (Univ. of Goettingen, Germany) "Subtleties and Surprises in Fluorinated Alcohol Clusters"
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> (Nominations for the next Vice Chair; Fill out Conference Evaluation Forms; Discuss future Site & Scheduling preferences; Election of the next Vice Chair)

7:30 pm - 9:30 pm	<b>DYNAMICS IN CLUSTERS</b>
7:30 pm - 7:45 pm	Overview by Discussion Leader: <b>Carl Lineberger</b> (Univ. of Colorado/JILA, USA)
7:45 pm - 8:30 pm	<b>David Nesbitt</b> (Univ. of Colorado/JILA, USA) "Intramolecular Dynamics in Molecular Ions: A High Resolution Perspective"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	<b>Takayuki Ebata</b> (Hiroshima Univ., Japan) "IVR Dynamics of the X-H Stretching Vibrations studied by Picosecond IR-UV Pump-Probe Spectroscopy"
9:20 pm - 9:30 pm	Discussion
9:45 pm -	Poster Session 3

## THURSDAY

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	<b>CLUSTERS CONTAINING BIOLOGICAL MOLECULES</b>
9:00 am - 9:15 am	Overview by Discussion Leader: <b>Mattanjah de Vries</b> (UC-Santa Barbara, USA) "What can we learn from isolating biomolecules in the gas phase?"
9:15 am - 10:00 am	<b>Tim Zwier</b> (Purdue Univ., USA) "Reorienting, shuttling, and dissociating water from a solute-water complex: New insights from hole-filling methods"
10:00 am - 10:10 am	Discussion
10:10 am	Coffee Break
10:40 am - 11:25 am	<b>Bernd Brutschy</b> (Univ. of Frankfurt, Germany) "Biomolecules in the Gas Phase by Laser Desorption/Ablation from Liquid Droplets"
11:25 am - 11:35 am	Discussion
11:35 am - 12:20 pm	<b>Klaus Mueller-Dethlefs</b> (Univ. of Manchester, UK) "TBA"
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>INTERMOLECULAR POTENTIALS</b>
7:30 pm - 7:45 pm	Overview by Discussion Leader: <b>Jeremy Hutson</b> (Univ. of Durham, UK) "Intermolecular potentials: the problem of excited states"
7:45 pm - 8:30 pm	<b>Wolfgang Domcke</b> (Tech. Univ. of Munich, Germany) "Cluster Models of Aqueous-Phase Photochemistry and the Solvated Electron"
8:30 pm - 8:40 pm	Discussion
8:40 pm - 9:20 pm	<b>Joel Bowman</b> (Emory Univ., USA) "Full dimensional <i>ab initio</i> potentials and quantum vibrational calculations for $\text{H}^+(\text{H}_2\text{O})_2$ , $\text{OH}^-(\text{H}_2\text{O})$ , and $\text{Cl}^-(\text{H}_2\text{O})$ "
9:20 pm - 9:30 pm	Discussion
9:45 pm -	Poster Session 4
<b>FRIDAY</b>	
7:30 am - 8:30 am	Breakfast
9:00 am	Depart

# MOLECULAR & IONIC CLUSTERS

Crowne Plaza  
Feb 19-24, 2006

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Name	Organization	Participation	Status
CHRISTIAN ADLHART	UNIVERSITY OF OSLO	Poster Presenter	Registered
DAVID T ANDERSON	UNIVERSITY OF WYOMING	Poster Presenter	Registered
ANTONIO ARMENTANO	UNIVERSITY OF MANCHESTER	Attendee	Registered
DARRIN BELLERT	BAYLOR UNIVERSITY	Poster Presenter	Registered
MARTIN BEYER	TU BERLIN	Poster Presenter	Registered
EVAN BIESKE	UNIVERSITY OF MELBOURNE	Poster Presenter	Registered
JOSEPH C BOPP	YALE UNIVERSITY	Poster Presenter	Registered
KIT H BOWEN	JOHNS HOPKINS UNIVERSITY	Speaker	Registered
JOEL BOWMAN	EMORY UNIVERSITY	Speaker	Registered
BERNHARD BRUTSCHY	UNIVERSITY OF FRANKFURT MAIN	Speaker	Registered
RALF U BURGERT	UNIVERSITAET KARLSRUHE	Poster Presenter	Registered
PROSSER D CARNEGIE	UNIVERSITY OF GEORGIA	Poster Presenter	Registered
A. WELFORD CASTLEMAN JR	PENNSYLVANIA STATE UNIVERSITY	Discussion Leader	Registered
CHRISTINE CEZARD	UNIVERSITY OF GOETTINGEN	Poster Presenter	Registered
MYONG YONG CHOI	DEPARTMENT OF CHEMISTRY	Poster Presenter	Registered
PRADYOT K CHOWDHURY	UNIVERSITY OF VICTORIA	Poster Presenter	Registered
MATTANJAH S DE VRIES	UNIVERSITY OF CALIFORNIA, SANTA BARBARA	Discussion Leader	Registered
WOLFGANG DOMCKE	TECHNICAL UNIVERSITY OF MUNICH	Speaker	Registered
OTTO DOPFER	UNIVERSITY OF WUERZBURG	Poster Presenter	Registered
GARY DOUBERLY	UNIVERSITY OF NORTH CAROLINA, CHAPEL HILL	Speaker	Registered
MICHAEL A DUNCAN	UNIVERSITY OF GEORGIA	Chair	Registered
TAKAYUKI EBATA	HIROSHIMA UNIVERSITY	Speaker	Registered
SOREN N EUSTIS	JOHNS HOPKINS UNIVERSITY	Poster Presenter	Registered
JOSEPH S FRANCISCO	PURDUE UNIVERSITY	Speaker	Registered
MASAAKI FUJII	TOKYO INSTITUTE OF TECHNOLOGY	Speaker	Registered
NARESH PATWARI GANPATHI	INDIAN INSTITUTE OF TECHNOLOGY BOMBAY	Attendee	Registered
DANIEL J GOEBBERT	PURDUE UNIVERSITY	Poster Presenter	Registered
GILLES GREGOIRE	LABORATOIRE PHYSIQUE DES LASERS CNRS	Poster Presenter	Registered
STEEN HAMMERUM	UNIVERSITY OF COPENHAGEN	Attendee	Registered
MARTINA HAVENITH	RUHR-UNIVERSITY BOCHUM	Speaker	Registered
JEFFREY M HEADRICK	YALE UNIVERSITY	Poster Presenter	Registered
JOHN M HERBERT	UNIVERSITY OF CALIFORNIA-BERKELEY	Poster Presenter	Registered
SAMANTHA HORVATH	THE OHIO STATE UNIVERSITY	Poster Presenter	Registered
JEREMY M HUTSON	UNIVERSITY OF DURHAM	Vice Chair	Registered
SHUN-ICHI ISHIUCHI	TOKYO INSTITUTE OF TECHNOLOGY	Poster Presenter	Registered
DAVID B P JACKSON	UNIVERSITY OF MANCHESTER	Poster Presenter	Registered
MARTIN F JARROLD	INDIANA UNIVERSITY	Speaker	Registered
MARK A JOHNSON	YALE UNIVERSITY	Speaker	Registered
KENNETH D JORDAN	UNIVERSITY OF PITTSBURGH	Discussion Leader	Registered
ASTER E KAMMRATH	UNIVERSITY OF CALIFORNIA, BERKELEY	Poster Presenter	Registered
WILLIAM KLEMPERER	HARVARD UNIVERSITY	Discussion Leader	Registered
ANNA I KRYLOV	UNIVERSITY OF SOUTHERN CALIFORNIA	Speaker	Registered
SANG HAK LEE	SEOUL NATIONAL UNIVERSITY	Poster Presenter	Registered
MARSHA I LESTER	UNIVERSITY OF PENNSYLVANIA	Speaker	Registered
XIANG LI	JOHNS HOPKINS UNIVERSITY	Poster Presenter	Registered
W. CARL LINEBERGER	UNIVERSITY OF COLORADO	Discussion Leader	Registered
JAMES M LISY	UNIVERSITY OF ILLINOIS, URBANA	Discussion Leader	Registered
ZHIFENG LIU	CHINESE UNIVERSITY OF HONG KONG	Poster Presenter	Registered

