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GORDON RESEARCH CONFERENCES *frontiers of science*
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Nancy Ryan Gray, Ph.D.
Director

2009 GORDON RESEARCH CONFERENCE
on
Electronic Spectroscopy and Dynamics
FINAL PROGRESS REPORT
DOE

DE-SC0000584

The Gordon Research Conference (GRC) on Electronic Spectroscopy and Dynamics was held at Colby College, Waterville, NH from 07/19/2009 thru 07/24/2009. The Conference was well-attended with 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In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field.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 As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings.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,

Mark Maroncelli
Penn State
University

Registration List

| Name | Organization | Participation |
|----------------------------|---------------------------------------|-------------------|
| Mark Maroncelli | PENN STATE UNIVERSITY | Chair |
| Timothy S. Zwier | PURDUE UNIVERSITY | Chair |
| Edward R. Grant | UNIVERSITY OF BRITISH COLUMBIA | Vice Chair |
| Bern Kohler | OHIO STATE UNIVERSITY | Vice Chair |
| Jeffrey A. Cina | UNIVERSITY OF OREGON | Discussion Leader |
| Yehuda Haas | HEBREW UNIVERSITY | Discussion Leader |
| Sam Leutwyler | UNIVERSITY OF BERN | Discussion Leader |
| Donald H. Levy | UNIVERSITY OF CHICAGO | Discussion Leader |
| Piotr Piotrowiak | RUTGERS UNIVERSITY | Discussion Leader |
| Paul F. Barbara | UNIVERSITY OF TEXAS AT AUSTIN | Speaker |
| David A. Blank | UNIVERSITY OF MINNESOTA | Speaker |
| Laurie J. Butler | UNIVERSITY OF CHICAGO | Speaker |
| Takayuki Ebata | HIROSHIMA UNIVERSITY | Speaker |
| Robert W. Field | MIT | Speaker |
| Carl C. Hayden | SANDIA NATIONAL LABORATORIES | Speaker |
| James T. Hynes | UNIVERSITY OF COLORADO | Speaker |
| David M. Jonas | UNIVERSITY OF COLORADO | Speaker |
| Scott Kable | UNIVERSITY OF SYDNEY | Speaker |
| John P. Maier | UNIVERSITY OF BASEL | Speaker |
| Richard A. Mathies | UNIVERSITY OF CALIFORNIA, BERKELEY | Speaker |
| Spiridoula Matsika | TEMPLE UNIVERSITY | Speaker |
| Frederic Merkt | ETH ZURICH | Speaker |
| David F. Plusquellic | NIST | Speaker |
| Hanna Reisler | UNIVERSITY OF SOUTHERN CALIFORNIA | Speaker |
| Gregory D. Scholes | UNIVERSITY OF TORONTO | Speaker |
| Benjamin J. Schwartz | UNIVERSITY OF CALIFORNIA, LOS ANGELES | Speaker |
| Lyudmila Slipchenko | PURDUE UNIVERSITY | Speaker |
| Timothy P. Softley | UNIVERSITY OF OXFORD | Speaker |
| John F. Stanton | UNIVERSITY OF TEXAS AT AUSTIN | Speaker |
| Jaime A. Stearns | AIR FORCE RESEARCH LAB | Speaker |
| Toshi Suzuki | KYOTO UNIVERSITY | Speaker |
| Wim Ubachs | VRIJE UNIVERSITEIT AMSTERDAM | Speaker |
| Thomas Udem | MAX PLANK INSTITUTE FOR QUANTENOPTIK | Speaker |
| Xiaoyang Zhu | UNIVERSITY OF TEXAS | Speaker |
| Leonardo Alvarez-Valtierra | UNIVERSIDAD DE GUANAJUATO | Poster Presenter |
| Jason D. Biggs | UNIVERSITY OF OREGON | Poster Presenter |
| Arthur E. Bragg | UCLA | Poster Presenter |
| Ksenia B. Bravaya | UNIVERSITY OF SOUTHERN CALIFORNIA | Poster Presenter |
| Kristin A. Briney | UNIVERSITY OF WISCONSIN - MADISON | Poster Presenter |
| Wybren J. Buma | UNIVERSITY OF AMSTERDAM | Poster Presenter |

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| Chandrima Chatterjee | YALE UNIVERSITY | Poster Presenter |
| Trevor L. Courtney | UNIVERSITY OF COLORADO | Poster Presenter |
| Kimberly D. De La Harpe | THE OHIO STATE UNIVERSITY | Poster Presenter |
| Mark Dethlefsen | UNIVERSITY OF OXFORD | Poster Presenter |
| Joseph J. Dillon | JOHNS HOPKINS UNIVERSITY | Poster Presenter |
| Michael B. Doyle | WAYNE STATE UNIVERSITY | Poster Presenter |
| Masaaki Fujii | TOKYO INSTITUTE OF TECHNOLOGY | Poster Presenter |
| Jakob Grilj | UNIVERSITY OF GENEVA | Poster Presenter |
| Brianna R. Heazlewood | UNIVERSITY OF SYDNEY | Poster Presenter |
| Leslie V. Herman | UNIVERSITY OF WISCONSIN - MADISON | Poster Presenter |
| Anat Kahan | THE HEBREW UNIVERSITY OF JERUSALEM , ISRAEL | Poster Presenter |
| Tim Kowalczyk | MASSACHUSETTS INSTITUTE OF TECHNOLOGY | Poster Presenter |
| Jan PHILIP. Kraack | PHILIPPS-UNIVERSITY OF MARBURG | Poster Presenter |
| Ryoji Kusaka | HIROSHIMA UNIVERSITY | Poster Presenter |
| Adrian W. Lange | OHIO STATE UNIVERSITY | Poster Presenter |
| Elin ANN. McCormack | OXFORD UNI | Poster Presenter |
| Jonathan P. Morrison | UNIVERSITY OF BRITISH COLUMBIA | Poster Presenter |
| Natalia S. Nagornova | EPFL | Poster Presenter |
| Josh J. Newby | PURDUE UNIVERSITY | Poster Presenter |
| Jaime Ortega Arroyo | UBC | Poster Presenter |
| Yoonsoo Pang | UNIVERSITY OF CALIFORNIA, BERKELEY | Poster Presenter |
| Lorena Piticco | ETH ZURICH | Poster Presenter |
| David Pratt | UNIVERSITY OF PITTSBURGH | Poster Presenter |
| Thomas J. Preston | UNIVERSITY OF WISCONSIN - MADISON | Poster Presenter |
| Christopher J. Rennick | UBC | Poster Presenter |
| Christian Rensing | UNIVERSITY OF KARLSRUHE | Poster Presenter |
| Chirantha P. Rodrigo | PURDUE UNIVERSITY | Poster Presenter |
| Durba Roy | THE PENNSYLVANIA STATE UNIVERSITY | Poster Presenter |
| Eric So | OXFORD UNIVERSITY | Poster Presenter |
| Daniel Sprecher | ETH ZURICH | Poster Presenter |
| Joseph E. Subotnik | TEL AVIV UNIVERSITY | Poster Presenter |
| Alexander N. Tarnovsky | BOWLING GREEN STATE UNIVERSITY | Poster Presenter |
| Mohamad Toutounji | UAE UNIVERSITY | Poster Presenter |
| Tyler P. Troy | UNIVERSITY OF SYDNEY | Poster Presenter |
| Alexander Vdovin | UNIVERSITY OF AMSTERDAM | Poster Presenter |
| Cesar R. Viteri | GEORGIA INSTITUTE OF TECHNOLOGY | Poster Presenter |
| Hailing Wang | ARIZONA STATE UNIVERSITY | Poster Presenter |
| Xiaolei Zhu | JOHNS HOPKINS UNIVERSITY | Poster Presenter |
| Xiujuan Zhuang | ARIZONA STATE UNIVERSITY | Poster Presenter |
| Peter C. Chen | SPELMAN COLLEGE | Attendee |
| Ezra Daniel | TEL AVIV UNIVERSITY | Attendee |
| John M. Herbert | OHIO STATE UNIVERSITY | Attendee |

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| Richard Hildner | ICFO - THE INSTITUTE OF PHOTONIC SCIENCES | Attendee |
| Timothy W. Schmidt | UNIVERSITY OF SYDNEY | Attendee |
| Timothy C. Steimle | ARIZONA STATE UNIVERSITY | Attendee |

The GRC on Electronic Spectroscopy & Dynamics showcases some of the most recent experimental and theoretical developments in electronic spectroscopy that probes the structure and dynamics of isolated molecules, molecules embedded in clusters and condensed phases, and bulk materials. Electronic spectroscopy is an important tool in many fields of research, and this GRC brings together experts having diverse backgrounds in physics, chemistry, biophysics, and materials science, making the meeting an excellent opportunity for the interdisciplinary exchange of ideas and techniques.

Topics covered in this GRC include high-resolution spectroscopy, biological molecules in the gas phase, electronic structure theory for excited states, multi-chromophore and single-molecule spectroscopies, and excited state dynamics in chemical and biological systems.

Active participation of postdoctoral researchers and graduate students is encouraged.

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 - 7:40 pm Welcome / Introductory Comments by GRC Site Staff

7:40 pm - 9:10 pm **Electronic Spectroscopy at High Resolution 1: Few-Atom Systems**

Discussion Leader: **Ed Grant** (The University of British Columbia)

7:40 pm - 8:15 pm **Thomas Udem** (Max Planck Institute for Quantum Optics)
"Femtosecond Frequency Combs and High Resolution Spectroscopy"

8:15 pm - 8:25 pm Discussion

8:25 pm - 9:00 pm **Wim Ubachs** (Free University of Amsterdam)
"Rydberg Spectroscopy in a Heavy Bohr Atom: H⁺H"

9:00 pm - 9:10 pm Discussion

MONDAY

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Electronic Spectroscopy at High Resolution 2: Larger Molecules & Interactions**

Discussion Leader: **Elliot Bernstein** (Colorado State University)

9:00 am - 9:35 am **Frédéric Merkt** (ETH Zurich)
"High-Resolution Spectroscopic Investigations of High Rydberg States and Electrostatic Trapping Experiments"

9:35 am - 9:45 am Discussion

9:45 am - 10:20 am **Tim Softley** (Oxford University)
"Molecular Rydberg States Interacting with Solid Surfaces: Dynamics and Field Effects"

10:20 am - 10:30 am Discussion

10:30 am - 11:00 am Coffee Break

11:00 am - 11:35 am **Robert Field** (MIT)
"Acetylene: Just Large Enough"

- 11:35 am - 11:45 am Discussion
- 11:45 am - 12:20 pm **John Maier** (University of Basel)
"Electronic Spectra of Carbon Chain Radicals and Ions"
- 12:20 pm - 12:30 pm Discussion
- 12:30 pm Group Photo / Lunch
- 1:30 pm - 4:00 pm Free Time
- 4:00 pm - 6:00 pm Poster Session A-1
- 6:00 pm Dinner
- 7:30 pm - 9:05 pm **Theory for Electronically Excited States**
Discussion Leader: **Jeffrey Cina** (University of Oregon)
- 7:30 pm - 8:05 pm **John Stanton** (University of Texas at Austin)
"Photoelectron Spectroscopy and Dynamics in the Nitromethane Anion"
- 8:05 pm - 8:15 pm Discussion
- 8:15 pm - 8:35 pm Hot Topic Talk: **Ksenia Bravaya** (University of Southern California)
"The Effect of H-bonding and π -Stacking Interactions on Ionization Energies of DNA Bases"
- 8:35 pm - 8:40 pm Discussion
- 8:40 pm - 9:00 pm Hot Topic Talk: **Lyudmila Slipchenko** (Purdue University)
"Electronic Excitations in the Condensed Phase: Theoretical Insights"
- 9:00 pm - 9:05 pm Discussion

TUESDAY

- 7:30 am - 8:30 am Breakfast
- 9:00 am - 12:30 pm **Excited-State Dynamics**
Discussion Leader: **Samuel Leutwyler** (University of Bern)
- 9:00 am - 9:35 am **Laurie Butler** (University of Chicago)
"Radical Intermediates of Bimolecular Reactions: Electronic and Nuclear Dynamics"
- 9:35 am - 9:45 am Discussion
- 9:45 am - 10:20 am **Hanna Reisler** (University of Southern California)
"Photodissociation Dynamics of Nitrogen Rich Molecules"
- 10:20 am - 10:30 am Discussion
- 10:30 am - 11:00 am Coffee Break
- 11:00 am - 11:35 am **Scott Kable** (University of Sydney)
"Reaction Dynamics in Aldehydes"
- 11:35 am - 11:45 am Discussion
- 11:45 am - 12:20 pm **Toshi Suzuki** (Kyoto University)
"Time-Resolved Photoelectron Imaging of Ultrafast Internal Conversion"
- 12:20 pm - 12:30 pm Discussion
- 12:30 pm Lunch
- 1:30 pm - 4:00 pm Free Time
- 4:00 pm - 6:00 pm Poster Session A-2
- 6:00 pm Dinner
- 7:30 pm - 9:30 pm **Biological Molecules in the Gas Phase**
Discussion Leader: **Donald Levy** (University of Chicago)
- 7:30 pm - 8:05 pm **Jaime Stearns** (Air Force Research Lab)

- 8:05 pm - 8:15 pm Discussion "Spectroscopy and Photodissociation of Cold, Protonated Peptides"
- 8:15 pm - 8:50 pm **Takayuki Ebata** (Hiroshima University)
"Laser Spectroscopy Studies of Functional Molecules"
- 8:50 pm - 9:00 pm Discussion

WEDNESDAY

- 7:30 am - 8:30 am Breakfast
- 9:00 am - 12:30 pm **Single-Molecule and Multi-Chromophore Systems**
Discussion Leader: **Piotr Piotrowiak** (Rutgers University)
- 9:00 am - 9:35 am **Carl Hayden** (CRF Sandia)
"Time-Resolved Multi-Spectral Single Molecule Spectroscopy"
- 9:35 am - 9:45 am Discussion
- 9:45 am - 10:20 am **Paul Barbara** (University of Texas at Austin)
"Single Molecule Spectroscopy Studies of the Charging and Discharging of Conjugated Polymers"
- 10:20 am - 10:30 am Discussion
- 10:30 am - 10:50 am Coffee Break
- 10:50 am - 11:25 am **David Blank** (University of Minnesota)
"Excited State Dynamics in Thiophene Oligomers, Dendrimers, and Polymers"
- 11:25 am - 11:35 am Discussion
- 11:35 am - 11:55 am Hot Topic Talk: **Richard Hildner** (ICFO Spain)
"Ultrafast Phase Controlled Excitation of Single Molecules"
- 11:55 am - 12:00 pm Discussion
- 12:00 pm - 12:20 pm Hot Topic Talk: **Timothy Schmidt** (University of Sydney)
"The Identification and Characterization of Resonance-Stabilized Hydrocarbon Radicals"
- 12:20 pm - 12:25 pm Discussion
- 12:30 pm Lunch
- 1:30 pm - 4:00 pm Free Time
- 4:00 pm - 6:00 pm Poster Session B-1
- 6:00 pm Dinner
- 7:00 pm - 7:30 pm Business Meeting
(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 - 9:00 pm **Multi-Chromophore Systems & Exciton Dynamics**
Discussion Leader: **Mark Maroncelli** (Penn State)
- 7:30 pm - 8:05 pm **Gregory Scholes** (University of Toronto)
"Electronic Coherence Despite Fast Dephasing: Energy Transfer and Two Exciton States"
- 8:05 pm - 8:15 pm Discussion
- 8:15 pm - 8:50 pm **Xiaoyang Zhu** (University of Minnesota)
"Exciton Formation and Dissociation at Semiconductor Interfaces"
- 8:50 pm - 9:00 pm Discussion

THURSDAY

- 7:30 am - 8:30 am Breakfast

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| 9:00 am - 12:30 pm | Electronic Coupling & Conical Intersections |
| | Discussion Leader: Yehuda Haas (Hebrew University of Jerusalem) |
| 9:00 am - 9:35 am | David Plusquellic (NIST) "Excitonic Interactions in Flexible Bichromophores" |
| 9:35 am - 9:45 am | Discussion |
| 9:45 am - 10:20 am | Spiridoula Matsika (Temple University) "The Role of Conical Intersections in the Photophysics of Biologically Relevant Molecules" |
| 10:20 am - 10:30 am | Discussion |
| 10:30 am - 11:00 am | Coffee Break |
| 11:00 am - 11:35 am | James Hynes (University of Colorado / Ecole Normale Superieure, Paris) "Polar Environmental Effects on Conical Intersection Structure and Dynamics" |
| 11:35 am - 11:45 am | Discussion |
| 11:45 am - 12:20 pm | David Jonas (University of Colorado) "Electronic Dynamics via Conical Funnels and Intersections" |
| 12:20 pm - 12:30 pm | Discussion |
| 12:30 pm | Lunch |
| 1:30 pm - 4:00 pm | Free Time |
| 4:00 pm - 6:00 pm | Poster Session B-2 |
| 6:00 pm | Dinner |
| 7:30 pm - 9:25 pm | Excited-State Dynamics in Solution |
| | Discussion Leader: Bern Kohler (Ohio State University) |
| 7:30 pm - 7:50 pm | Hot Topic Talk: John Herbert (Ohio State University) "Excited-State Quantum Chemistry for Macromolecules and Condensed Phases" |
| 7:50 pm - 7:55 pm | Discussion |
| 7:55 pm - 8:30 pm | Benjamin Schwartz (University of California at Los Angeles) "Watching the Solvation of Atoms in Liquids, One Solvent Molecule at a Time" |
| 8:30 pm - 8:40 pm | Discussion |
| 8:40 pm - 9:15 pm | Richard Mathies (University of California at Berkeley) "Femtosecond Stimulated Raman Spectroscopy (FSRS) of Excited State Photochemistry in Phytochrome and Green Fluorescent Protein (GFP): Picking Apart the Reaction Coordinate" |
| 9:15 pm - 9:25 pm | Discussion |
| FRIDAY | |
| 7:30 am - 8:30 am | Breakfast |
| 9:00 am | Depart |