
GENERAL INFORMATION

Internet Access. There is complimentary wi-fi access in the Administration Building.

Meals at Asilomar. For attendees lodging at Asilomar you will receive a meal ticket for all meals beginning with dinner on Friday and ending with lunch on Tuesday. For attendees staying off-site you will receive lunch tickets for Saturday, Sunday and Monday. Off-site lodgers wishing to purchase breakfast or dinner meal tickets may purchase them at the Asilomar Conference Center registration area in the Administration Building.

To-Go Lunches at Asilomar. Should you wish to take your lunch to the beach, please go to the regular lunch window and request a “To-Go Lunch”.

Program Overview.

Friday	Evening Session	7:15 – 9:30 pm
Saturday	Morning Sessions	9:00 – 11:50 am
	Afternoon Session	1:00 – 3:40 pm
	Evening Session	7:15 – 9:30 pm
Sunday	Morning Session	9:00 – 11:50 am
	Free Afternoon	
	Evening Session	7:15 – 9:30 pm
Monday	Morning Session	9:00 – 11:50 am
	Afternoon Session	1:00 – 4:15 pm
	Banquet	6:00 – 7:15 pm
	After-Dinner Talk	7:15 – 8:00 pm

Poster Presenters. Please mount your poster display on Friday before 7:00 pm or during the evening reception, 8:30 – 9:30 pm. Boards are numbered. See poster list on page 9 to learn your assigned board space.

Speakers. Please arrive in the Chapel, session room, 15 minutes prior to the start of the session to set up your laptop computer.

Survey. You will receive an email with a link to the online conference survey. Your feedback is appreciated.

Sunday Afternoon. There is a free afternoon scheduled for Sunday. Please see page 11 of this program for some suggested activities or visit the Front Desk/Administration Hall building where many maps and brochures are available.

CONFERENCE SPONSOR

Banquet Wine Sponsor
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CONFERENCE INTRODUCTION

Ion Spectroscopy

The 2009 Asilomar conference will focus on ion spectroscopy, broadly defined. The continuing emergence of new and improved light sources, coupled with steadily advancing mass spectrometer technology, has given a renaissance in spectroscopy of gas-phase ions. New generations of synchrotron light sources in the UV and innovations in IR sources (free electron lasers, benchtop OPO lasers) are being combined with novel ion generation and detection approaches such as velocity imaging and cryogenic ion traps. The conference aims to meld developments in the spectroscopy and mass spectrometry communities.

FRIDAY, OCTOBER 16, 2009

- 3:00 pm** **Guest Room Check-in**, *Asilomar Main Lobby*
- 4:00 – 6:00 pm** **Conference Registration**, *Asilomar Main Lobby*
- 6:00 – 7:00 pm** **Asilomar dinner for on-site lodgers**, *Crocker Dining Hall.*
Asilomar meal ticket required.

Evening presenters should arrive in the Chapel (session room) by 7:00 pm to set up laptops.

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- 7:15 – 8:30 pm** **Opening Session**, *Chapel*
Session Chair: Robert C. Dunbar
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- 7:15 – 7:20 pm Opening Remarks
- 7:20 – 7:55 pm **Michael A. Duncan**, *University of Georgia*
Cation IR Spectra Over a Wide Range: Hydrocarbons, Metal Carbonyls
- 7:55 – 8:30 pm **Cheuk-Yiu Ng**, *University of California, Davis*
Spectroscopy and Dynamics of Neutrals and Ions by High-Resolution
VUV and IR-VUV Laser Photoion-Photoelectron Methods
- 8:30 – 9:30 pm** **Informal Reception and Poster Viewing**

Posters should be set-up prior to 7:00 pm or during the reception.

SATURDAY, OCTOBER 17, 2009

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers**, *Crocker Dining Hall*.
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) at 8:45 am to set up laptops.

9:00 – 10:10 am **Infrared and Computations**, *Chapel*
Session Chair: Peter Armentrout

9:00 – 9:35 am **Gilles Ohanessian**, *CNRS, Ecole Polytechnique*
Progress Toward the Accurate Modelling of IR Spectra of
Oligopeptides

9:35 – 10:10 am **Bela Paizs**, *DKFZ, Heidelberg*
Structure of Peptide Fragments from Computational and IR Studies

10:10 – 10:40 am Coffee Break **and** Group Photo

10:40 – 11:50 am **Water**, *Chapel*
Session Chair: Evan Williams

10:40 – 11:15 am **Mark A. Johnson**, *Yale University*
Shape, Function and Reactivity of Water Clusters

11:15 – 11:50 am **Evan Williams**, *University of California, Berkeley*
What Hydrated Ionic Clusters Can Tell Us About Ions in Aqueous Solution

12:00 pm – 1:00 pm **Asilomar Lunch for all participants**, *Crocker Dining Hall*.
Asilomar meal ticket required.

Afternoon presenters should arrive in the Chapel (session room) by 12:45 pm to set up laptops.

1:00 – 2:10 pm **Photoionization I**, *Chapel*
Session Chair: Balint Sztaray

1:00 – 1:35 pm **Katharine Reid**, *University of Nottingham*
Challenging ZEKE: Applications of Photoelectron Velocity Map
Imaging at High Resolution

1:35 – 2:10 pm **Laurent Nahon**, *SOLEIL Synchrotron*
Valence-shell Photoelectron Circular Dichroism on Gas Phase Pure
Enantiomers Studied with Imaging PEPICO Techniques

2:10 – 2:40 pm Coffee Break

2:40 – 3:40 pm **Hot Topics I, Chapel**
Session Chair: Chip Cody

2:40 – 3:00 pm Jeffrey D. Steill, *FOM Institute for Plasma Physics ‘Rijnhuizen’*
Spectroscopically-Resolved Competition Between Dissociation and
Electron Detachment from Nitrobenzene and Other Molecular Anions

3:00 – 3:20 pm Mathias Schäfer, *University of Cologne*
Infrared Multiphoton Dissociation Spectroscopy of Cationized Proline
and N-Methyl Alanine: Effects of Alkali-Metal Cation Size on Gas-
Phase Conformation

3:20 – 3:40 pm Jana Roithova, *Charles University, Prague*
Ground-state Reactivity of Hydrocarbon Dications and Their Nitrogen
Analogues towards Methane

6:00 – 7:00 pm **Asilomar dinner for on site lodgers, Crocker Dining Hall.**
Asilomar meal ticket required.

Evening presenters should arrive in *Chapel* by 7:00 pm to set up laptops.

7:15 – 8:25 pm **Infrared I, Chapel**
Session Chair: Nick Polfer

7:15 – 7:50 pm **Gary Groenewold**, *Idaho National Laboratory*
IRMPD Studies of Uranyl Coordination Complexes

7:50 – 8:25 pm **Gerard Meijer**, *Fritz-Haber-Institut*
Metal Clusters, Metal-oxides and Cluster-adsorbate Complexes

8:25 – 9:30 pm **Informal Reception and Poster Viewing**

SUNDAY, OCTOBER 18, 2009

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers**, *Crocker Dining Hall*.
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) by 8:45 am to set up laptops.

9:00 – 10:10 am **Photoionization II**
Session Chair: Tom Baer

9:00 – 9:35 am **Ivan Powis**, *University of Nottingham*
Vibrational Effects in Photoionization Spectroscopy, with Particular
Reference to Circular Dichroism Measurements

9:35 – 10:10 am **Andras Bödi**, *Paul Scherrer Institut*
First Results from the iPEPICO Endstation at the Swiss Light Source:
The Surprisingly Complex Spectroscopy and Dissociation Dynamics of
Small Molecules

10:10 – 10:40 am Coffee Break

10:40 – 11:50 am **UV / Visible**
Session Chair: Richard Cole

10:40 – 11:15 am **Ricardo Metz**, *University of Massachusetts*
Electronic and Vibrational Spectroscopy of Intermediates of C-H:
Activation by Metal and Metal-Oxide Cations

11:15 – 11:50 am **John P. Maier**, *University of Basel*
Electronic Spectroscopy of Astrophysically Relevant Ions

12:00 pm – 1:00 pm **Asilomar Lunch for all participants**, *Crocker Dining Hall*.
Asilomar meal ticket required.

1:00 – 6:00 pm **Free Time**, *please see page XX for sightseeing activities.*

6:00 – 7:00 pm **Asilomar dinner for on site lodgers**, *Crocker Dining Hall*
Asilomar meal ticket required.

SUNDAY EVENING, OCTOBER 18, 2009

Evening presenters should arrive in the Chapel (session room) at 7:00 pm to set up laptops.

7:15 – 8:25 pm **Infrared II**
Session Chair: John Eyler

7:15 – 7:50 pm **Thomas Rizzo**, *EPFL Lausanne*
Conformation-specific Vibrational Spectroscopy of Cold, Biomolecular Ions

7:50 – 8:25 pm **Mary T. Rodgers**, *Wayne State University*
Probing the Effects of Cationization on the Structures of a Variety of Nucleobases, Model Phosphate Esters and the 2'-deoxymononucleotide-5'-phosphates by IRMPD and Theory

8:25 – 9:30 pm **Informal Reception and Poster Viewing**

MONDAY, OCTOBER 19, 2009

7:30 – 9:00 am **Asilomar Breakfast for on-site lodgers**, *Crocker Dining Hall*.
Asilomar meal ticket required.

Morning presenters should arrive in the Chapel (session room) at 8:45 am to set up laptops.

9:00 – 11:50 am **Different Approaches**
Session Chair: Vicki H. Wysocki

- 9:00 – 9:35 am **Joel H. Parks**, *Rowland Institute at Harvard*
Dynamics of Non-covalent Complexes and Small Proteins via
Measurements of Fluctuations
- 9:35 – 10:10 am **Frank Turecek**, *University of Washington*
SERS Spectra of Soft-landed Ions
- 10:10 – 10:40 am Coffee Break
- 10:40 – 11:15 am **Dong-Sheng Yang**, *University of Kentucky*
Metal Binding to Gas-phase Nucleobases from ZEKE and IR-UV
Spectroscopy
- 11:15 – 11:50 am **Rebecca A. Jockusch**, *University of Toronto*
Gas-phase Ion Photodissociation and Photon Emission in the
Visible/Ultraviolet Region
- 12:00 – 1:00 pm** **Asilomar lunch for all participants**, *Crocker Dining Hall*.
Asilomar meal ticket required.

Afternoon presenters should arrive in the Chapel (session room) by 12:45 pm to set up laptops.

1:00 – 3:15 pm **Infrared III**
Session Chair: Travis Fridgen

- 1:00 – 1:35 pm **Evan Bieske**, *University of Melbourne*
Cold Complexes and Hot Particles – Mixing Laser Spectroscopy and
Mass Spectrometry
- 1:35 – 2:10 pm **Jos Oomens**, *FOM Rijnhuizen*
Anion Spectroscopy at FELIX
- 2:10 – 2:40 pm Coffee Break
- 2:40 – 3:15 pm **Philippe Maitre**, *CLIO Orsay*
Gas Phase IR Spectroscopy of Inorganic and Organometallic
Complexes

3:15 – 4:15 pm Hot Topics II
Session Chair: Detlef Schroeder

3:15 – 3:35 pm **James S. Prell**, *University of California, Berkeley*
Microsolvation of Protonated Phenylalanine and Phenylalanine Derivatives: Competition between Binding Sites Revealed by Hydrogen-Stretch IRPD Spectroscopy

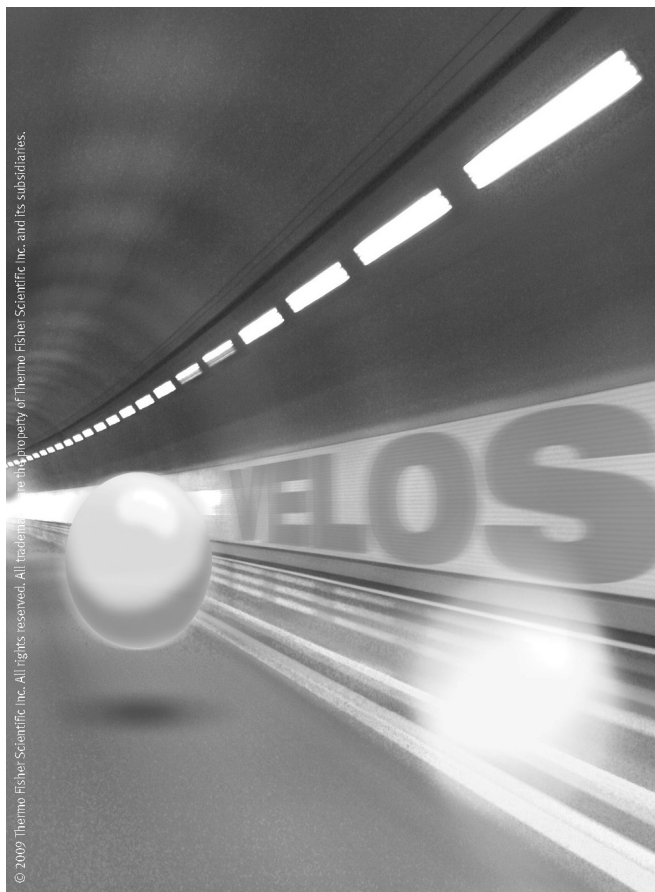
3:35 – 3:55 pm **Nicolas C. Polfer**, *University of Florida*
Telling Carbohydrate Isomers Apart: Ir Photodissociation Spectroscopy of Metal-Tagged Glucuronic and Iduronic Acid

3:55 – 4:15 pm **John R. Eyler**, *University of Florida*
Differentiation of Mono- And Disaccharide Structures with Infrared Multiple Photon Dissociation Spectroscopy

6:00 – 7:00 pm Banquet, Seascape Room. Banquet ticket required.
Wine served at the Banquet is sponsored by Thermo Scientific.

7:15 – 8:00 pm After-Dinner Speaker, Chapel.
Eric Herbst, *The Ohio State University*
Positive and Negative Molecular Ions Throughout the Universe
Dessert will be served following the talk.

Thank you Thermo Scientific, sponsor of Banquet Wine.



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POSTERS

Board

- 1 **Peter B. Armentrout**, *University of Utah*; Infrared Multiphoton Dissociation Spectroscopy of Cationized Cysteine and Methionine: Effects of Alkali-Metal Cation on Gas-Phase Conformation
- 2 **Michael Burt**, *Memorial University of Newfoundland*; Structures of [Pb(AminoAcid-H)]⁺ complexes Using Infrared Multiple Photon Dissociation
- 3 **Vanessa A. Castleberry**, *Baylor University*; The Low Energy Unimolecular Reaction Rate Constants for the Gas Phase, Ni⁺-Mediated Dissociation of the C-C Σ -Bond in Acetone And (D₆)-Acetone
- 4 **Richard B. Cole**, *University of New Orleans*; Laser-Induced Oxidation of Cholesterol as Observed by MALDI-TOF Mass Spectrometry
- 5 **Robert C. Dunbar**, *Case Western Reserve University*; A Beautiful Ion Cage: Metal Ion Complexes with PhePhe
- 6 **Ashley C. Gucinski**, *University of Arizona*; Action IRMPD Spectroscopy for Structural Determination of a Set His containing b₂⁺ Ions
- 7 **Christopher L. Hendrickson**, *NHMFL, Florida State University*; Gas Phase Ion Structure Determination at the National High Magnetic Field Laboratory
- 8 **Chow-shing Lam**, *University of California, Davis*; Rovibronically Selected and Resolved Two-Color Laser Photoionization and Photoelectron Study of the Iron Carbide Cation
- 9 **Yawei Lin**, *University of Ottawa*; Participation of O₂ Shumann -Runge Bands in keV CID Experiments
- 10 **Alexandre Loboda**, *MDS Analytical Technologies*; UV Photodissociation of Complex Organic Ions in a Pressurized Linear Ion Trap
- 11 **Matthew Meyer**, *University of Minnesota*; Utilizing Photoelectron Imaging to Probe the Structure of Cyclopropenyl Anions
- 12 **Warren K. Mino**, *University of Florida*; Measuring Infrared “Fingerprint” Spectra of Gas-Phase Zwitterions Using a Continuous Wave OPO Laser
- 13 **Christopher Moss**, *University of Washington*; Are DFT Methods Reliable for Assigning Peptide Ion Structures?
- 14 **Laurent Nahon**, *Synchrotron SOLEIL*; Synchrotron Radiation for Tandem Mass Spectrometry
- 15 **Jeremy T. O’Brien**, *University of California, Berkeley*; Charge Solvated and Salt Bridge Structures of Halidated Amino Acids: Results from IRMPD Spectroscopy and Theory
- 16 **James S. Prell**, *University of California, Berkeley*; IRPD Spectroscopy of Extensively Hydrated Ions: Understanding Ion Hydration and the Water Surface
- 17 **James Redwine**, *Purdue University*; A Novel Tandem Mass Spectrometer for the Spectroscopic Characterization of Cold Biomolecular Ions
- 18 **Detlef Schroeder**, *Institute of Organic Chemistry and Biochemistry*; Comments on the Assignment of Isomeric Using IRMPD Spectra
- 19 **Xiaoyu Shi**, *University of California, Davis*; Rovibronically Selected and Resolved Two-color Laser PFI-PE Study of Nickel Carbide
- 20 **William R. Stevens**, *University of North Carolina at Chapel Hill*; Dissociative Photoionization Study of Neopentane: A path to an Accurate Heat of Formation of the t-butyl Ion
- 21 **Bálint Sztáray**, *University of Pacific*; iPEPICO Studies on the Energetics of Atmospherically Relevant S_xO_yCl_z Ions