

Dynamics of Molecular Collisions 2013 Schedule

Sunday, July 7

Arrival and Registration

4:00 - 6:00 pm, Registration, Mountain-Lake Room

6:00 - 7:30 pm, Dinner, Garden Deck

7:30 - 10:00 pm, Reception, Garden Deck

Monday, July 8

7:30 - 8:30: Breakfast, Granhall

Bimolecular Reactions I, Mountain-Lake Room

8:30 - 8:45: Session Overview: *Kopin Liu* (Academia Sinica)

8:45 - 9:15: *David Clary* (U. Oxford), Combining Quantum Dynamics and Quantum Chemistry for Reactions of Polyatomic Molecules

9:15 - 9:25: Discussion

9:25 - 9:55: *Xueming Yang* (Dalian Institute of Chemical Physics), Reagent Vibrational Excitation Effect on the Dynamics of the F+HD Reaction

9:55 - 10:05: Discussion

10:05 - 10:50: Coffee break

10:50 - 11:20: *Tim Minton* (Montana State U.) , Electronic Excitation in Hyperthermal Atomic Oxygen Reactions

11:20 - 11:30: Discussion

11:30 - 11:45: Contributing talk: *Baptiste Joalland* (Wayne State U.), Crossed-beam Slice Imaging of Cl Reaction Dynamics with Butene Isomers

11:45 - 11:50: Discussion

11:50 - 12:20: *Zhigang Sun* (Dalian Institute of Chemical Physics), State-to-state Reactive Scattering by MCTDH Method

12:20 - 12:30: Discussion

12:30 - 2:00: Lunch, Garden Deck

2:00 - 4:30: Free (set up posters, odd numbers)

4:30 - 5:30: Poster Session (odd numbers), Bay Room

5:30 - 7:00: Dinner, Garden Deck

Non-adiabatic Dynamics, Mountain-Lake Room

7:00 - 7:15: Session Overview, *Spiridoula Matsika* (Temple U.)

7:15 - 7:45: *David Yarkony* (Johns Hopkins U.), Electronic Structure Aspects of Nonadiabatic Dynamics: Reaction Mechanisms and Representations of Coupled Adiabatic States

7:45 - 7:55: Discussion

- 7:55 - 8:25: *John Tully* (Yale U.), Chemical Dynamics at Metal Surfaces: The Role of Electronic Excitations
- 8:25 - 8:35: Discussion
- 8:35 - 8:50: Break
- 8:50 - 9:05: Contributing talk, *J. Jankunas* (Stanford U.), Simultaneous Measurement of Reactive and Inelastic Scattering of $H + HD \rightarrow HD(v', j') + H$ Reaction: In Search for Geometric Phase Effects
- 9:05 - 9:10: Discussion
- 9:10 - 9:40: *Anna Krylov* (U. Southern California), On the Photodetachment from the Green Fluorescent Protein Chromophore
- 9:40 - 9:50: Discussion
- 9:50 - 12:00: Poster session (odd numbers), Bay Room

Tuesday, July 9

- 7:30 - 8:30: Breakfast, Granhall

Unimolecular Reactions, Mountain-Lake Room

- 8:30 - 8:45: Session Overview: *Wen Li* (Wayne State U.)
- 8:45 - 9:15: *Don Truhlar* (U. Minnesota), Photochemistry in Terms of Diabatic States
- 9:15 - 9:25: Discussion
- 9:25 - 9:55: *Dan Neumark* (U. California Berkeley), Probing Chemical Dynamics with Negative Ions
- 9:55 - 10:05: Discussion
- 10:05 - 10:50: Coffee break
- 10:50 - 11:20: *Andrei Sanov* (U. Arizona), Radical and Diradical Reactive Intermediates via Anion Photoelectron Imaging
- 11:20 - 11:30: Discussion
- 11:30 - 11:45: Contributing talk: *Michael Lucas* (U. California Riverside), Ultraviolet Photodissociation Dynamics of the Cyclohexyl Radical
- 11:45 - 11:50: Discussion
- 11:50 - 12:20: *Bob Continetti* (U. California San Diego), Studies of Neutral Reaction Dynamics using Dissociative Photodetachment: HCO_2 and $F + H_2O \rightarrow HF + OH$
- 12:20 - 12:30: Discussion
- 12:30 - 2:00: Lunch, Garden Deck
- 2:00 - 4:30: Free
- 4:30 - 5:30: Poster Session (odd numbers), Bay Room
- 5:30 - 7:00: Dinner, Garden Deck

Cold Collisions, Mountain-Lake Room

- 7:00 - 7:15: Session Overview: *Stefan Willitsch* (U. Basel)
- 7:15 - 7:45: *Pascal Honvault* (U. Franche-Comté), Quantum Reaction Dynamics Studies of Astrophysical Interest below 100 K

- 7:45 - 7:55: Discussion
- 7:55 - 8:25: *Bas van de Meerakker* (Radboud U.), Controlling Collisions using Stark-decelerated Molecular Beams
- 8:25 - 8:35: Discussion
- 8:35 - 8:50: Break
- 8:50 - 9:05: Contributing talk, *Heather Lewandowski* (JILA), Travelling-Wave Deceleration of Buffer-Gas Beams of CH
- 9:05 - 9:10: Discussion
- 9:10 - 9:40: *Jeremy Hutson* (Durham U.) Ultracold Hydrogen Atoms: A Versatile Coolant for Producing Microkelvin Molecules
- 9:40 - 9:50: Discussion
- 9:50 - 12:00: Poster session (odd numbers)

Wednesday, July 10

- 7:30 - 8:30: Breakfast, Granhall

Interface Dynamics, Mountain-Lake Room

- 8:30 - 8:45: Session Overview: *Rainer Beck* (EPF Lausanne)
- 8:45 - 9:15: *David Nesbitt* (JILA/U. Colorado), Probing Gas-Liquid and Gas-SAM Interfaces with Quantum State Resolved Collision Dynamics
- 9:15 - 9:25: Discussion
- 9:25 - 9:55: *Bret Jackson* (U. Mass. Amherst), Dynamics of Methane Dissociation on Ni and Pt Surfaces
- 9:55 - 10:05: Discussion
- 10:05 - 10:50: Coffee break
- 10:50 - 11:20: *Alec Wodtke* (U. Göttingen/MPI), Charge Transfer Reactions Induce Born-Oppenheimer Breakdown in Surface Chemistry: Applications of Double Resonance Spectroscopy in Molecule-surface Scattering
- 11:20 - 11:30: Discussion
- 11:30 - 11:45: Contributing talk: *Bin Jiang* (U. New Mexico), Mode/Bond Selectivity in Methane Dissociative Chemisorption on Ni(111)
- 11:45 - 11:50: Discussion
- 11:50 - 12:20: *Geert-Jan Kroes* (Leiden U.), Towards a Chemically Accurate Description of Reactive Molecule-surface Scattering
- 12:20 - 12:30: Discussion
- 12:30 - 2:00: Lunch, Garden Deck
- 2:00 - 4:30: Free (set up posters, even numbers), Bay Room
- 4:30 - 5:30: Poster Session (even numbers), Bay Room
- 5:30 - 7:00: Dinner, Garden Deck

Bimolecular Reactions II, Mountain-Lake Room

- 7:00 - 7:15: Session Overview: *Al Wagner* (Argonne National Lab)
7:15 - 7:45: *Bill Hase* (Texas Tech U.), Simulations of $X^- + CH_3Y$ Ion-Molecule Reactions. Roles of Non-Statistical Dynamics, Multiple Reaction Pathways, and Microsolvation
7:45 - 7:55: Discussion
7:55 - 8:25: *Arthur Suits* (Wayne State U.), Rydberg Tagging of Spin-Polarized Hydrogen Atoms
8:25 - 8:35: Discussion
8:35 - 8:50: Break
8:50 - 9:05: Contributing talk, *Gábor Czako* (Eötvös U.) Dynamics of Bimolecular Polyatomic Reactions on Ab Initio Potential Energy Surfaces
9:05 - 9:10: Discussion
9:10 - 9:40: *Uwe Manthe* (U. Bielefeld), Quantum Dynamics of Methane-Atom Reactions
9:40 - 9:50: Discussion
9:50 - 12:00: Poster session (even numbers), Bay Room

Thursday, July 11

- 7:30 - 8:30: Breakfast, Granhall

Clusters and Solution Reactions, Mountain-Lake Room

- 8:30 - 8:45: Session Overview: *Marsha Lester* (U. Pennsylvania)
8:45 - 9:15: *Andrew Orr-Ewing* (U. Bristol), Vibrationally Resolved Dynamics and Energy Flow for Reactions in Solution
9:15 - 9:25: Discussion
9:25 - 9:55: *P.-N. Roy* (U. Waterloo), Dynamics of Quantum Rotors in Complex Environments
9:55 - 10:05: Discussion
10:05 - 10:50: Coffee break
10:50 - 11:20: *Fleming Crim* (U. Wisconsin Madison) Dissociation and Isomerization in Clusters and Solution
11:20 - 11:30: Discussion
11:30 - 11:45: Contributing talk: *Diane Lancaster* (U. Wisconsin Madison), Inert Gas Scattering from Liquid Hydrocarbon Microjets
11:45 - 11:50: Discussion
11:50 - 12:20: *Tim Zwier* (Purdue U.) Multiple Resonance Methods for Conformation-Specific Spectroscopy and Dynamics
12:20 - 12:30: Discussion

12:30 - 2:00: Lunch, Garden Deck
2:00 - 4:30: Free
4:30 - 5:30: Poster Session (even numbers), Bay Room
5:30 - 7:00: Dinner, Garden Deck

Award Session, Mountain-Lake Room

- 7:00 - 7:10: Introduction: *Dave Chandler* (Sandia National Lab), *Arthur Suits* (Wayne State U.) and *Hua Guo* (U. New Mexico)
- 7:10 - 7:50: *Giacinto Scoles* (U. Udine), Chemical Dynamics of Complex Reactions with Biomolecules: the Case of Restriction Enzymes in Highly Packed DNA Brushes
- 7:50 - 8:00: Discussion
- 8:00 - 8:40 *Peter Toennies* (MPI Göttingen), Superfluid Helium Droplets: Some New Results and Insights.
- 8:40 - 8:50: Discussion
- 8:50 - 9:30: *Joel Bowman* (Emory U.), Potential Energy Surfaces
- 9:30 - 9:40: Discussion
- 9:40 - 12:00: Poster session (even numbers), Bay Room

Friday, July 12

- 7:30 - 8:30: Breakfast, Granhall

Atmospheric, Astrochemical, and Combustion Reactions, Mountain-Lake Room

- 8:30 - 8:45: Session Overview: *Richard Dawes* (Missouri U. Sci. Tech.)
- 8:45 - 9:15: *Ralf Kaiser* (U. Hawaii Manoa), On the Formation of Interstellar Organosilicon Molecules
- 9:15 - 9:25: Discussion
- 9:25 - 9:55: *Hanna Reisler* (U. Southern California), Imaging Bond Breaking in Hydrogen-bonded Dimers and Trimers
- 9:55 - 10:05: Discussion
- 10:05 - 10:50: Coffee break
- 10:50 - 11:20: *David Osborn* (Sandia National Lab) Isomers and Isomerizations in Tropospheric Chemistry: Opening the Black Box of Criegee Intermediate Reactions
- 11:20 - 11:30: Discussion
- 11:30 - 11:45: Contributing talk: *Julia Lehman* (U. Pennsylvania), Photodissociation Dynamics of the Simplest Criegee Intermediate CH₂OO and its Laboratory Precursor CH₂I₂
- 11:45 - 11:50: Discussion
- 11:50 - 12:20: *Kristie Boering* (U. California Berkeley) Reaction Dynamics and Kinetics of Oxygen Isotope Exchange Reactions: Insights into Unusual Isotope Effects and Their Applications in Earth and Planetary Science
- 12:20 - 12:30: Discussion
- 12:30 - 1:30: Lunch, Garden Deck
- 1:30: Conference adjourns