

Sunday, July 6

3:00 pm-6:00 pm Check-in and badge pickup

6:00 pm-7:30 pm Dinner

7:30 pm-9:00 pm Welcome and Keynote Address

7:30 pm-7:45 pm Welcome by **Amy Mullin** (University of Maryland)

7:45 pm-8:00 pm Keynote Introduction by **Art Utz** (Tufts University)

8:00 pm-8:45 pm Keynote Address by **Alec Wodtke** (Max Planck Institute for Multidisciplinary Science and Institute for Physical Chemistry, Göttingen)
“A Golden Age of Quantitative Chemistry: Experiment, Theory and the Dynamics of Molecular Collisions”

8:45 pm-9:00 pm Discussion

9:00 pm Reception

Monday July 7

7:00 am-8:10 am Breakfast

8:10 am-12:00 pm Bimolecular Collision Dynamics

8:10 am-8:25 am Session Introduction: **Stephen Klippenstein** (Argonne National Laboratory)

8:25 am-8:55 am **Richard D Thomas** (Stockholm University)
“Probing molecular mutual neutralization reactions of atmospheric importance using the ion storage facility DESIREE”

8:55 am-9:05 am Discussion

9:05 am-9:35 am **Jennifer Meyer** (RPTU Kaiserslautern-Landau)
“Dynamics of CO₂ action by transition metal ions: Competition between spin-changing and spin-conserving pathways”

9:35 am- 9:45 am	Discussion
9:45 am-10:05 am	Andrew Petit (California State University, Fullerton) “New Insights into the Electronic Quenching of NO* with Acetylene: Energy Transfer Versus the Harpoon Mechanism”
10:05 am- 10:10 am	Discussion
10:10 am-10:40 am	<u>Coffee Break</u>
10:40 am-11:10 am	Richard Dawes (Missouri University of Science and Technology) “Methods for PES Construction with Applications: Typical and Special Cases, Diabatization, and the Long Range”
11:10 am-11:20 am	Discussion
11:20 am- 11:50 am	Arthur Suits (University of Missouri) “New Probes of Kinetics and Spectroscopy in Supersonic Flows”
11:50 am-12:00 pm	Discussion
12:00 pm-1:00 pm	<u>Lunch</u>
1:00 pm-5:00 pm	Afternoon Break
5:00 pm-6:00 pm	Hot Topic Poster Previews Greta Jacobson (University of Washington) “Machine Learning Approaches for Developing Potential Surfaces: Applications to OH-(H ₂ O) _n (n=1-4) Complexes” Yang Liu (University of New Mexico) “Kinetics and Product Branching in Dihydrogen Activation by Gaseous Manganese Oxide Cations” Olivia Krohn (Sandia National Laboratory) “Ultrahigh Velocity Resolution for Inelastic Scattering Dynamics” Chow Shing Lam (University of Oxford) “Probing the Ultrafast Dynamics of Nitrobenzene through Time-Resolved Coulomb Explosion Imaging” Chao He (University of Basel) “Exploring the Chemi-ionization of Carbonyl Sulfide (OCS) with Metastable Neon via Velocity Map Imaging”

John Hack (University of California, Berkeley)
 “Coherent Vibrations in C-I Bond Dissociation Studied with Carbon K-edge Transient Absorption”
Simone DeSouza (University of Maryland)
 “Dynamics of Optically Centrifuged N₂O in Extreme Rotational States Studied with Transient IR Absorption Spectroscopy”
Madison Foreman (University of California, Berkeley)
 “Molecular Beam Scattering from Flat Liquid Jets: Exploring Dynamics at the Aqueous Interface”

6:00-7:15 pm Dinner

7:15 pm-9:30 pm Collision Dynamics in the Condensed Phase

7:15 pm- 7:30 pm Session Introduction: **Stephen Bradforth** (University of Southern California)

7:30 pm-8:00 pm **Ward Thompson** (University of Kansas)
 “Activation Energies Beyond Arrhenius”

8:00 pm-8:10pm Discussion

8:10 pm-8:40 pm **Chris Elles** (University of Kansas)
 “Ultrafast Dynamics of Manganese Tricarbonyl Coordination Complexes”

8:40 pm-8:50 pm Discussion

8:50 pm-9:20 pm **Graham Worth** (University College London)
 “Simulating Non-adiabatic in Photo-excited Reactions using Direct Quantum Dynamics”

9:20 pm-9:30 pm Discussion

9:30 pm Poster Session 1 (A posters)

Tuesday, July 8

7:00 am-8:10 am Breakfast

8:10 am – 12:00 pm Photodissociation Dynamics

8:10 am-8:25 am	Session Introduction: Marsha Lester (University of Pennsylvania)
8:25 am-8:55 am	Mike Duncan (University of Georgia) “Infrared and UV-Visible Photodissociation of Organometallic Cations”
8:55 am- 9:05 am	Discussion
9:05 am-9:35 am	Daniel Neumark (University of California, Berkeley) “Photodissociation dynamics investigated using XUV and soft x-ray attosecond transient absorption”
9:35 am-9:45 am	Discussion
9:45 am-10:05 am	Joseph McManus (University of Oxford) “Tracking ultrafast structural change in photoexcited cis and trans isomers”
10:05 am-10:10 am	Discussion
10:10 am-10:40 am	<u>Coffee Break</u>
10:40 am-11:10 am	Katharine Tibbetts “Ultrafast Photodissociation Dynamics in Energetic Molecules”
	Discussion
11:20-11:50 am	Jingsong Zhang “Isomer selected photochemistry of C ₄ H ₇ radicals”
11:50 am-12:00 pm	Discussion
12:00 pm- 1:00 pm	Lunch
1:00 pm-5:00 pm	Afternoon Break
5:00 pm-7:15 pm	Dynamics and Potential Energy Surfaces- In honor of David Yarkony
5:00 pm-5:15 pm	Session Introduction: Hua Guo (University of New Mexico)
5:15 pm-5:45 pm	Spiridoula Matsika (Temple University) “Modeling Ultrafast Excited State Dynamics”

5:45 pm-5:55 pm	Discussion
5:55 pm- 6:25 pm	Michael Schuurman (University of Ottawa) “The UV Absorption and Time-Resolved Spectroscopy of Ethylene: A New Theoretical Model”
6:25 pm – 6:35 pm	Discussion
6:35 pm-7:05 pm	Benjamin Levine (Stonybrook University) “First Principles Simulation of Coherent Dynamics on Many Electronic States”
7:05 pm-7:15 pm	Discussion
7:15 pm-8:15 pm	Dinner
8:15 pm	Poster Session 2 (A posters)

Wednesday, July 9	
7:00 am-8:10 am	Breakfast
8:10 am-12:00 pm	Dynamics of Interfacial Collisions
8:10 am-8:25 am	Session Introduction by Art Utz (Tufts University)
8:25-8:55 am	David Nesbitt (JILA, University of Colorado) “Making a Splash: Chemical Physics at the Gas-Liquid Interface”
8:55 am-9:05 pm	Discussion
9:05 am-9:35 am	Theofanis Kitsopoulos “Applying Ion Imaging Methods to Site Specific Elementary Reactions in Heterogeneous Catalysis”
9:35 am-9:45 am	Discussion
9:45 am-10:05 am	Mihai E. Vaida “Facet-Dependent Ultrafast Photoinduced Reaction Dynamics of CH ₃ I on TiO ₂ Surfaces”

10:05 am-10:10 am	Discussion
10:10 am-10:40 am	<u>Coffee Break</u>
10:40 am-11:10 am	G. Barratt Park (Texas Tech University) “State-to-State Scattering of Open Shell Atoms from Surfaces”
10:10 am-10:20 am	Discussion
11:20 am-11:50 am	George Schatz (Northwestern University) “Nonadiabatic Dynamics and Ionization in N+ N and N + O Collisions”
11:50 am - 12:00 pm	Discussion
12:00 pm – 1:00 pm	Lunch
1:00 pm – 5:00 pm	Afternoon Break
5:00 pm – 6:00 pm	Business Meeting
6:00 pm – 7:15 pm	Dinner
7:15 pm - 9:30 pm	Herschbach Medal Session
7:15 pm-7:30 pm	Session Introduction: Arthur Suits (University of Missouri)
7:30 pm-7:45 pm	Introduction of David Chandler: Mark Johnson (Yale University)
7:45 pm-8:30 pm	David W. Chandler (Sandia National Laboratory) “Measuring Velocity With High Resolution for Low Energy Molecules and Electrons”
8:30 pm-8:45 pm	Introduction of Anne McCoy: Mark Johnson (Yale University)
8:45 pm-9:30 pm	Anne B. McCoy (University of Washington) “Deciphering spectral signatures of proton delocalization in complexes of hydroxide and hydronium ions with water molecules”
9:30 pm	Poster Session 3 (B posters)

Thursday, July 10

7:00 am-8:10 am Breakfast

8:10 am-12:00 pm **Spectroscopy, dynamics, and electronic structure: In honor of John Stanton**

8:10 am-8:25 am Session Introduction: **Anne McCoy** (University of Washington)

8:25 am - 8:55 am **Jan Martin** (University of Florida)
“Exploiting a Shortcoming of Coupled-Cluster Theory: The Extent of non-Hermiticity as a Diagnostic Indicator of Computational Accuracy”

8:55 am-9:05 am Discussion

9:05 am-9:35 am **Rigoberto Hernandez** (Johns Hopkins University)
“Classical and Semiclassical Transition State Theory: Old and New”

9:35 am-9:45 am Discussion

9:45 am-10:05 am **Yaolong Zhang** (University of New Mexico)
SchrödingerNet: A Universal Neural Network Solver for The Schrödinger Equation

10:05 am-10:10 am Discussion

10:10 am-10:40 am Coffee Break

10:40 am-11:10 am **David Tannor** (Weizman Institute of Science)
“Two Hundred Years after Hamilton: Exploring New Formulations of Classical and Quantum Mechanics”

10:10 am-11:20 am Discussion

11:20 am-11:50 am **Carolyn Anna Joy** (Marquette University)
“Recent Advances in Mixed Quantum/Classical Theory (MQCT) for Molecule + Molecule Collisions”

11:50 am-12:00 pm Discussion

12:00 pm -1:00 pm Lunch

1:00 pm-5:00 pm	Afternoon Break
5:00 pm-7:15 pm	Quantum Control of Reaction Dynamics
5:00 pm-5:15 pm	Session Introduction: Amy Mullin
5:15 pm-5:45 pm	Marissa Weichman (Princeton University) “New Platforms for Molecular Polariton Dynamics”
5:45 pm-5:55 pm	Discussion
5:55 pm-6:25 pm	Helen Chadwick (Swansea University) “Rotationally controlled hydrogen-surface reactions”
6:25 pm-6:35 pm	Discussion
6:35 pm-7:05 pm	Yu Liu (University of Maryland) “Advancing reaction dynamics with ultracold molecules”
7:05 pm-7:15 pm	Discussion
7:15 pm-8:15 pm	Dinner
8:15 pm	Poster Session 4 (B posters)

Friday, July 11

7:00 am-8:10 am	Breakfast
8:10 am - 8:25 am	Applications of Molecular Collision Dynamics
8:10 am-8:15 am	Session Introduction: Ahren Jasper (Argonne National Laboratory)
8:25 am-8:55 am	Robert Continetti (University of California, San Diego) “Hypervelocity Ice Grain Impact Mass Spectrometry and the Search for Extraterrestrial Biosignatures”
8:55 am-9:05 am	Discussion
9:05 am-9:35 am	Arkke Eskola (University of Helsinki)

	“Direct Kinetic Studies of Unimolecular and Bimolecular Reactions of Criegee Intermediates”
9:35 am-9:45 am	Discussion
9:45 am-10:05 am	Shane Goettl (University of Hawaii) “Gas-Phase Synthesis of Cyclic Silicon Dicarbide (c-SiC ₂) and Bicyclic Silicon Tricarbide (c-SiC ₃) via Single Collision Events from Acyclic Transients”
10:05 am-10:10 am	Discussion
10:10 am-10:40 am	<u>Coffee Break</u>
10:40 am-11:10 am	Denisia Popolan-Vaida (University of Central Florida) “Influence of Carbon Chain Length, Functionality, and Reaction Environment on C1-C7 Criegee Intermediates Reaction Networks”
11:10 am-11:20 am	Discussion
11:20 am-11:50 am	Brandon Rotavera (University of Georgia) “Bimolecular Reactions of Cyclic Ether Radicals”
11:50 am-12:00 pm	Discussion
12:00 pm-12:05 pm	Thanks and DMC XXX Ahren Jasper
12:05 pm-1:30 pm	Box lunches in lobby outside lecture hall