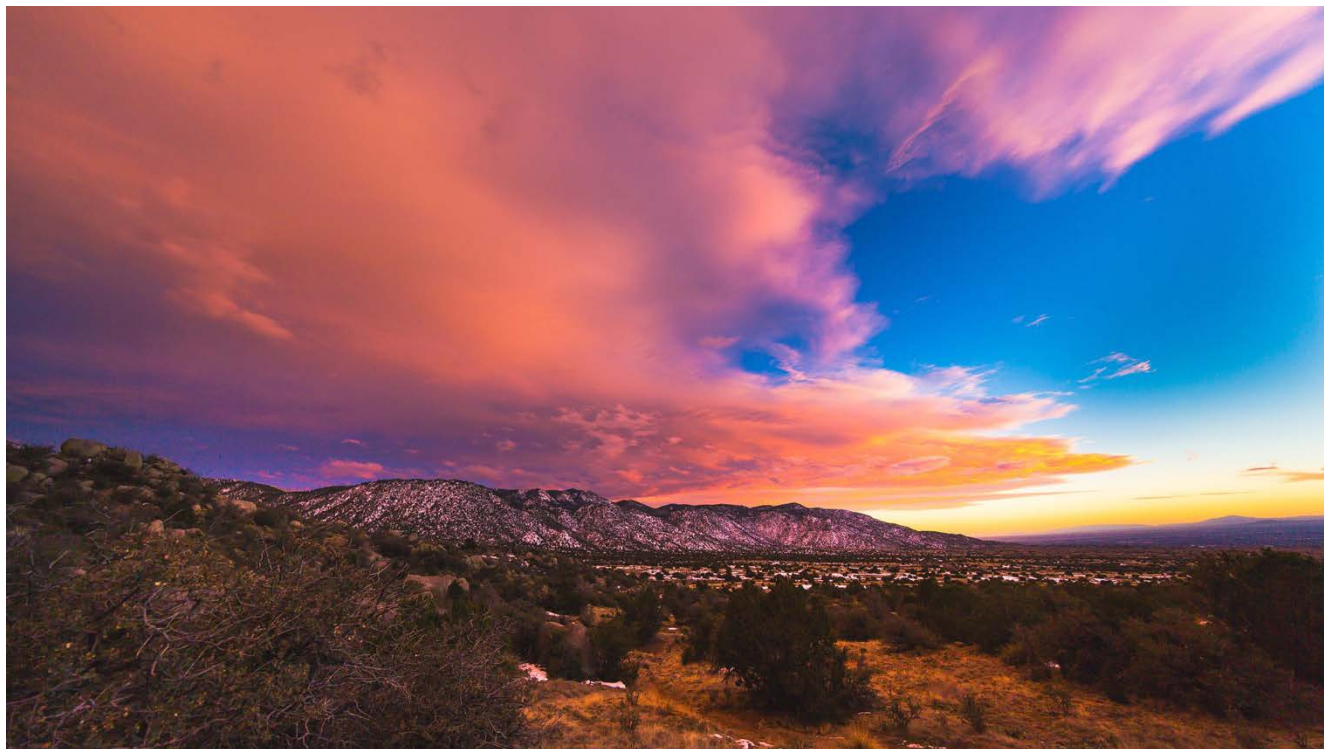


# *39th Reaction Mechanisms Conference*



*June 23-26, 2024*  
*University of New Mexico*  
*Albuquerque, New Mexico*

*Chairs: Kathleen Morgan and William Karney*  
*Local Organizer: Brian Gold*

*Thanks to Sponsors for Support of this RMC*

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~~of chemical research~~



*Journal of* **Physical  
Organic Chemistry**



## **RMC – General Information for Attendees**

**Check-in:** Sunday June 23, 2-6PM, UNM Student Union Building (SUB), outside of Ballroom C. If you bought a parking pass, you can pick it up at this time. If you need to park while registering on Sunday, you can park in any official parking spot that's not reserved and not on a meter. If you are arriving on Monday, there is a Visitor Parking area or metered parking on Redondo Rd close to the SUB where you can park for a small fee.

An annotated campus map is included at the end of the full program.

The conference welcome and first session begin Sunday 6/23 at 6PM in SUB Ballroom C. Talks end Wednesday 6/26 at 1PM.

The University of New Mexico is a walking-intensive campus located in the high desert a mile above sea level. Participants with limited mobility may wish to contact the organizers for more information. It is recommended that all participants drink lots of water to stay hydrated! Hats and sunscreen are recommended as well. There are large temperature swings from day to night, and being prepared for temperatures ranging from 60-100+ is advisable.

**Food:** The conference will be providing the following:

Sunday and Monday poster sessions: heavy appetizers and cash bar

Monday, Tuesday and Wednesday mornings: coffee/tea and light pastries at 8AM, and coffee break at 10:15AM

Conference dinner on Tuesday, with one drink ticket followed by cash bar

Other meals are not included. The SUB has a couple food vendors open during the day, and a grab-and-go vendor. The main campus dining hall, La Posada, is also open and is a 5-minute walk from the SUB. The door rates there are \$9.25 for breakfast and \$11.15 for lunch/dinner, both plus tax. There are several restaurants within a short walk of the SUB as well.

**Poster Sessions:** There are two scheduled poster sessions (Sun 8:05-10:00pm and Mon 4-6pm) with a total of 34 posters. The structure is informal, meaning that presenters are NOT assigned to a particular session. Rather, we hope poster presenters will attend and consider presenting at both sessions, and use some of the time to view other posters. The posters can be set up by Sunday at 8pm (possibly earlier?), and should remain up through Monday at 6pm. The poster area is in the Student Union Building, outside Ballroom C.

### **Staying Safe on Campus**

UNM is an open campus situated in a thriving metropolitan area of Albuquerque. UNM is committed to offering services, information, resources and tools to support a safe campus to all students, staff, faculty, and visitors. We encourage individuals to contribute to campus safety and preparedness by becoming informed, staying alert and using good judgment. More detailed safety recommendations are included in the email message sent to all attendees.

In the event of a building alarm, participants must evacuate according to posted signage and maintain a distance of at least 50 feet from the building, re-entering only at the approval of staff.

**Dorm Housing:** Check-in is Sunday June 23, 2-6PM at the Student Union Building outside of Ballroom C, together with conference check-in. The dorms (Laguna or DeVargas) are a 5-minute walk from the Student Union Building. We can help with bags if needed. The room will have sheets, towels, and a pillow. You need to bring all personal care items.

Check-out is 7:30-11AM on Wednesday June 26 at the dorms. For those attending the excursion on Wednesday, we have reserved a room in the SUB for you to store your bags in the Student Union Building if needed, until after the excursion.

**Parking:** If you signed up for a parking pass, there are two R lots near the dorm that you can use.

24-hour dorm help desk: (505) 277-2606

**Late arrival or early departure:** If you arrive after 6PM Sunday, you can check in at the 24-hour housing desk, in the Student Residence Center, building 89. If you need to check out before 7:30AM on Wednesday 6/26, please bring your key here as well.

Alcohol and overnight guests are prohibited in the dorms. More detailed information on dorm policies is in the email message sent to those staying in the dorms.

## **Meeting Program**

### **SUNDAY, June 23**

2:30-6:00 pm      **Arrival and Check-in** (Student Union Building, outside Ballroom C)

6:00-6:10 pm      **Welcome and Introductory Remarks** (Student Union Building, Ballroom C)

### **Photochemistry and Polymers**

*Discussion Leader: Dean Tantillo (University of California, Davis)*

6:10-6:45 pm      **Samuel Leguizamon** (Sandia National Laboratory)  
Photocontrol of Olefin Metathesis Polymerizations via Ruthenium Catalyst Inhibition

6:45-7:20 pm      **Veronica Vaida** (University of Colorado, Boulder)  
Pyruvic Acid Multiphase Photochemistry from Gas and Aqueous Phases to the Water-Air Interface

7:20-7:55 pm      **Erin Stache** (Princeton University)  
Photon Driven Strategies for Activating Strong Bonds for Polymer Recycling Applications

7:55-8:05 pm      **Remembrance of Josef Michl**

8:05-10:00 pm     **Poster Session 1**

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### **MONDAY, June 24**

### **Environmental Chemistry & Photochemistry**

*Discussion Leader: Julie Peterson (Bowling Green State University)*

8:30-9:05 am      **AnGayle Vasiliou** (Middlebury College)  
Thermal Cracking of Hydrocarbons: A Molecular Viewpoint

9:05-9:40 am      **Joseph Francisco** (University of Pennsylvania)  
Catalytic and Autocatalytic Mechanisms in the Atmospheric Chemistry Context

9:40-10:15 am     **Javier Read de Alaniz** (University of California, Santa Barbara)  
Exploration of Light Responsive Materials

10:15-10:30 am    Coffee break

## Earth-Abundant Metal Catalysis

*Discussion Leader: Sheryl Wiskur (University of South Carolina)*

- 10:35-11:10 am **Annaliese Franz** (University of California, Davis)  
Structure and Mechanistic Insight into New Aminoamide Silanol Ligands for Cu-Catalyzed Enantioselective N-H Insertion Reactions
- 11:10-11:45 am **Maren Podewitz** (TU Wien / Vienna University of Technology)  
Catalysis in Confinement: Mechanism and Dynamics of C-X Bond Formation with Supramolecular Catalysts
- 11:45-12:20 pm **Sam Yruegas** (Rice University)  
Mechanistic Insights towards Calcium-Mediated Functionalization
- 12:20-1:30 pm (Lunch on your own)
- 1:30-2:20 pm **Undergraduate Context Session**  
*Moderator: Jason Gillmore*  
For undergraduates to meet and ask questions about the science presented so far at RMC.
- 2:30-3:20 pm **Industry Panel: Applying Your Mechanistic Toolbox Toward Problems in Industrial Research**  
*Moderator: Thomas Peterson*  
A presentation and discussion on how those with mechanistic backgrounds can make important and unique contributions in industrial research.
- 4:00-6:00 pm **Poster Session 2**

## Enzymes and Biological Mechanisms

*Discussion Leader: Lesley-Ann Giddings (Smith College)*

- 7:00-7:35 pm **Zhongyue (John) Yang** (Vanderbilt University)  
Reasons to Be Cool: How Do Enzymes Remain Active at Low Temperatures
- 7:35-8:10 pm **Judith Klinman** (University of California, Berkeley)  
An Emerging Dynamical Mechanism for the Thermal Activation of Enzyme Activity
- 8:10-8:45 pm **Changjian Feng** (University of New Mexico)  
Deciphering Nitric Oxide Synthase Isozyme Regulation through Conformational Dynamics
- 8:45-9:20 pm **Ivan Castillo** (Universidad Nacional Autónoma de México)  
Monooxygenase-Inspired Reactive Copper-Oxygen Intermediates Supported by Benzimidazole Ligands
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TUESDAY, June 25

## Late Transition Metal Catalysis

*Discussion Leader: Alexander Greer (Brooklyn College of the City University of New York)*

- 8:30-9:05 am      **Sharon Neufeldt** (Montana State University)  
Mechanistic Origin of Selectivity in Pd-Catalyzed Cross-Coupling
- 9:05-9:40 am      **Nilay Hazari** (Yale University)  
Understanding the Mechanism of Ni-Catalyzed Cross-Electrophile Coupling Reactions
- 9:40-10:15 am     **Paulami Majumdar** (Dow Inc.)  
Heterogeneous Catalysts for Ethylene Carbonylation
- 10:15-10:30 am    Coffee break

## Theory, Excited States, and Carbocations

*Discussion Leader: Jeehiun Lee (Rutgers University)*

- 10:35-11:10 am    **Angela Wilson** (Michigan State University)  
Building Control of Reaction Mechanisms: Excitation and Deexcitation Pathways
- 11:10-11:45 am    **Alison Frontier** (University of Rochester)  
Iterative Cationic Cyclizations for the Synthesis of Polycyclic Targets
- 11:45-12:20 pm    **Rigoberto Hernandez** (Johns Hopkins University)  
Transition State Theory for Chemical Reactions in Complex Environments
- 12:20-1:30 pm     (Lunch on your own)
- 1:30-2:20 pm      **Diversity Session: Inclusive Practices in Challenging Times**  
A brief overview of three successful initiatives at Xavier University of Louisiana.  
Participants are encouraged to share their experiences.

## Tribute to Cynthia Burrows

*Discussion Leader: Barry Carpenter (Cardiff University)*

- 3:00-3:05 pm      **Tribute Welcome**
- 3:05-3:40 pm      **Steve Rokita** (Johns Hopkins University)  
Revealing the Mechanism of a Flavin-Dependent Reductive Dehalogenase Using the Principles of Organic Chemistry
- 3:40-4:15 pm      **Sheila David** (University of California, Davis)  
Mysteries of MUTYH: Base Excision Mechanism, Metal Cofactors and Implications for Medicine

- 4:15-4:50 pm      **Vahe Bandarian** (University of Utah)  
Leveraging Radical Enzymatic Chemistry Towards Biotechnology
- 4:50-5:30 pm      **RMC Honoree: Cynthia Burrows** (University of Utah)  
Taming Free Radical Oxidation of DNA to Control Gene Expression
- 5:30-9:00 pm      **Reception and Conference Dinner** (Student Union Building, Ballroom B)
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**WEDNESDAY, June 26**

### **From Data Science to Decarboxylations**

*Discussion Leader: Robert McMahon (University of Wisconsin, Madison)*

- 8:30-9:05 am      **Ajit Vikram** (Merck Inc.)  
Data-Rich Experimentation for Reaction Kinetic Investigation of Pharmaceutically Relevant Processes
- 9:05-9:40 am      **Jolene Reid** (University of British Columbia)  
Data-Driven Mechanistic Modeling of Asymmetric Catalysis
- 9:40-10:15 am      **Richard O'Hair** (University of Melbourne)  
Adventures With the Pesci Decarboxylation Reaction: From Synthesis, Structure, and Reactivity of Organometallics to Development of New Transfer Hydroarylation Isodesmic Reactions for Organic Synthesis
- 10:15-10:30 am      Coffee break

### **Carbocations and Carbon Catalysts**

*Discussion Leader: Richard Johnson (University of New Hampshire, National Science Foundation)*

- 10:35-11:10 am      **Steven Kass** (University of Minnesota)  
Development of Weakly Coordinating Cations: What Happens If Opposites Don't Attract?
- 11:10-11:45 am      **Paul Rablen** (Swarthmore College)  
Are CN (and a Few Other EWG's) Really meta-Directors in Electrophilic Aromatic Substitution?
- 11:45-12:20 pm      **O. Maduka Ogba** (Chapman University)  
Heteroallene Reduction by Zerovalent Carbon Catalysts
- 12:20-12:55 pm      **Yiming Wang** (University of Pittsburgh)  
Cationic Late Transition Metal Complexes for Selective alpha-C-H Functionalization
- 12:55-1:00 pm      **Closing Remarks**
- 1:15 pm              **Excursion** (bus leaves for Sandia Tramway)  
(Box lunches provided for excursion participants)
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**List of Posters - Informal Structure (no assigned sessions for presenters; all posters on display)****Poster Session 1: Sunday, June 23, 8:05-10:00 pm****Poster Session 2: Monday, June 24, 4:00-6:00 pm**

1	<b>Siraj Z. Ali</b>	Massachusetts Institute of Technology	Nitration of Carboxylic Acids by P <sup>III</sup> /P <sup>V</sup> -Catalysis
2	<b>Arslan Atangulov</b>	New Mexico State University	Computational Investigation of the SN2 Reaction Mechanism in Transphosphorylation of the DUSP5 Protein
3	<b>Donald H. Aue</b>	University of California, Santa Barbara	Reaction Dynamics for Rearrangements of Cyclobutylidene
4	<b>Donald H. Aue</b>	University of California, Santa Barbara	Dynamics for Rearrangements of Bicyclic Cyclobutylidenes
5	<b>Vincent Conrad Oppenheimer</b>	University of Colorado, Denver	The use of sodium hypochlorite pentahydrate as an effective chlorinating agent of benzo[ <i>b</i> ]thiophene derivatives
6	<b>S. Sooriyage Dulanjali, Victoria Nisoli</b>	University of New Mexico	Expanding the Protein Bioconjugation Toolbox Targeting Gla Residues on Gla Proteins
7	<b>Lesley-Ann Giddings</b>	Smith College	Characterization of a Broadly Specific Cadaverine <i>N</i> -Hydroxylase involved in Desferrioxamine B Biosynthesis in <i>Streptomyces sviveus</i>
8	<b>Brian Gold</b>	New Mexico State University	Push–Pull Cyclooctyne Dimerizations
9	<b>Alexander Greer</b>	Brooklyn College, The Graduate Center of the City College of New York	Shrinking the Molecular Gap: Improved Mechanistic Understanding of Phototruncation Through Physical Organic Chemistry
10	<b>Dagoberto Grijalva-Flores</b>	University of Colorado, Denver	Synthesis of the Phosphoramidite of 8-oxo-7,8-Dihydroguanosine to Establish the Structural Impact of 8-oxoG on Tetraloop Hairpins of RNA
11	<b>Jordan L. Harper</b>	Los Alamos National Laboratory	Computational Investigation into the Regioselective Formation of 2,5-Diketopiperazines
12	<b>Michael J. Holzmann</b>	University of New Mexico	Twist to React: Tuning Linked Biaryl Cyclononynes for Molecular Applications
13	<b>Waseem Hussain</b>	New York University	Aziridination via Nitrogen-Atom Transfer to Olefins from Photoexcited Azoxy-Triazenes
14	<b>James E. Jackson</b>	Michigan State University	Could vibrational dipolar interactions or directional dispersion explain alkane/perfluoroalkane immiscibility?
15	<b>Ishika Jain</b>	University of San Francisco	Heavy-Atom Tunneling in Cascade Electrocyclizations in the Biosynthesis of Natural Products
16	<b>Said Jalife</b>	University of Houston	Modulating Paratropicity in Polycyclic Antiaromatic Hydrocarbons
17	<b>Philip P. Lampkin</b>	University of Wisconsin–Madison	Bifunctional Dihydrazone Catalysts for Rapid Foldamer-templated Aldol Condensation Reactions

18	<b>Jesse LePluart</b>	University of New Mexico	Investigating the Effects of Geometric and Electronic Structure on <i>Formate Dehydrogenase</i> Reactivity
19	<b>Kathleen M. Morgan</b>	Xavier University of Louisiana	A Computational Study of the Gas-Phase Behavior of Substituted Epoxide Radicals
20	<b>Keaton Mulshine, J. Henry Westphal</b>	Hope College	More Robust Long-Wavelength BF <sub>2</sub> -Azo Dyes?
21	<b>Amanda Nilsen</b>	University of San Francisco	Computational Study of Heavy-Atom Tunneling in Biosynthesis: Model Systems for the Cope Rearrangement
6	<b>Victoria Nisoli, S. Sooriyage Dulanjali</b>	University of New Mexico	Expanding the Protein Bioconjugation Toolbox Targeting Gla Residues on Gla Proteins
22	<b>Julie Peterson</b>	Bowling Green State University	Revisiting an Old Photoswitch: Isomerization of Stenhouse Salts in Protic Solvents
23	<b>Emmanuel Quartey</b>	University of New Mexico	Mechanistic Insights into Glyoxyl-Derived Isomers of Arginine
24	<b>Claire Scott, Alison Wegner</b>	Hope College	LC/UV-vis and LC/MS/MS to study the retinal carotenoids of songbirds as a factor of habitat and diet
25	<b>Paul H. Scudder</b>	New College of Florida	Generate and Select: Installing a Rule-based Organic Expert System on Students
26	<b>Wook Shin</b>	Vanderbilt University	Entropy Mediates Ambimodal Selectivity of Cycloadditions
27	<b>C. J. Stephenson</b>	Loyola University New Orleans	Understanding the Ring Opening Mechanism of Rhodamine and Aziridine Based Sensors and Switches
28	<b>Alexandra Strom</b>	Smith College	Mechanism of Iron-Catalyzed Oxidative Amination of Ketones
29	<b>Gerald Tanoury</b>	Vertex Pharmaceuticals Inc.	An AIMD Study on Amine Nitrosation by N <sub>2</sub> O <sub>3</sub> and N <sub>2</sub> O <sub>4</sub> in Explicit Water
30	<b>Thomas Tao</b>	Skidmore College	Tandem Intramolecular Diels-Alder/1,3-Dipolar Cycloaddition in the Synthesis of the Vinca Alkaloids
31	<b>James I. Vesto</b>	University of California, Davis	Targeted Organosilanol Ligand Development for Asymmetric Catalysis of an N-H Insertion Reaction
24	<b>Claire Scott, Alison Wegner</b>	Hope College	LC/UV-vis and LC/MS/MS to study the retinal carotenoids of songbirds as a factor of habitat and diet
20	<b>J. Henry Westphal, Keaton Mulshine</b>	Hope College	More Robust Long-Wavelength BF <sub>2</sub> -Azo Dyes?
32	<b>Sheryl Wiskur</b>	University of South Carolina	How Intermolecular Interactions Rule Organocatalysis
33	<b>Zeng Rong Wong</b>	University of California, Berkeley	Difluorocarbene Insertion into the Metal-Carbon Bond: Suppressing $\alpha$ -Fluoride Elimination with a Gold(I) System
34	<b>Jing Yang</b>	University of New Mexico	The Mitochondrial Amidoxime Reducing Component (mARC) is not a Canonical Sulfite Oxidase Family Enzyme