

Crushing Chemistry

❖ NSF Center for the Mechanical Control of Chemistry ❖

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CMCC Scholars Successfully Defend Their Doctoral Theses



Katie Floyd



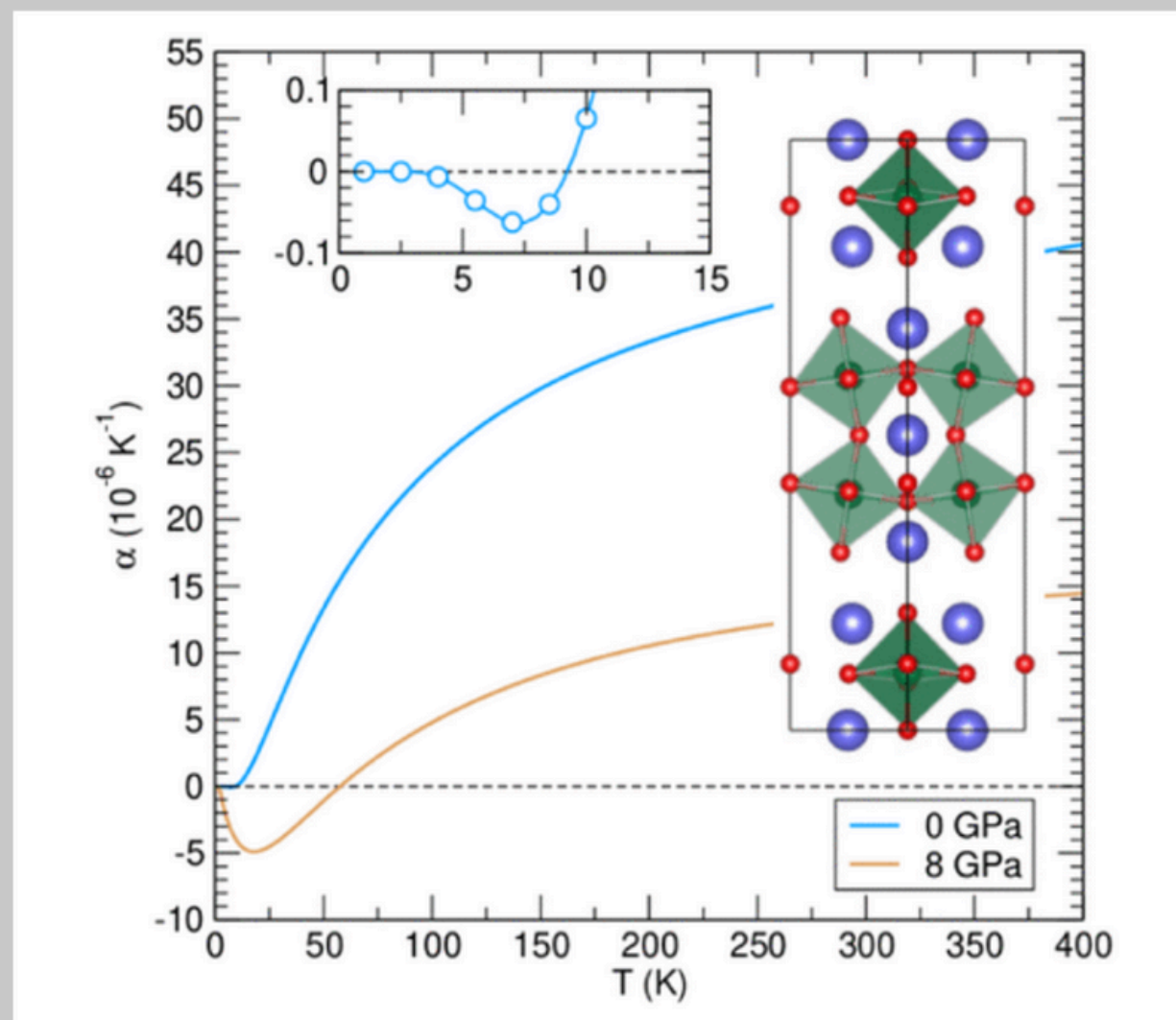
Eric Riesel



Rohesh Silva

The CMCC proudly celebrates three exceptional scholars who have successfully defended their doctoral theses. Katie Floyd (left), a graduate student in the Batteas lab at *Texas A&M University*, has successfully defended her doctoral thesis and earned her PhD in Chemistry. Eric Riesel (middle), a graduate student in the Freedman group at *MIT*, has successfully defended his doctoral thesis and earned his PhD in Chemistry. Rohesh Silva (right), a graduate student in the Mack group at the *University of Cincinnati*, has successfully defended his doctoral thesis and earned his PhD in Organic Chemistry. Congratulations Katie, Eric, and Rohesh on your remarkable accomplishments! We look forward to the impact you will continue to make in your respective fields.

New Publication in *Inorganic Chemistry*



Koocher, N. Z., Altman, A. B., Klein, R. A., Malliakas, C. D., Jacobsen, S. D., Freedman, D. E., & Rondinelli, J. M. (2025). Tunable Negative Thermal Expansion in Layered Perovskite Ba₃Zr₂S₇. *Inorganic chemistry*.



Researchers from the Altman, Rondinelli, and Freedman Groups of the CMCC have reported a new discovery in materials science, focusing on the layered perovskite sulfide Ba₃Zr₂S₇. Their study, published in *Inorganic Chemistry*, reveals that this material exhibits tunable negative thermal expansion (NTE) at low temperatures, a property where the material contracts upon heating.

The team used computational methods to predict this pressure-tunable NTE, which stems from a quasi-2D vibration mechanism. This finding suggests new avenues for designing materials with tailored thermal properties, particularly for applications in conventional photovoltaic devices, where controlling thermal expansion is crucial for performance and durability.

To learn more, scan the QR code.

Probing Mechanochemical Reactions at Sliding Interfaces by Ab Initio and Machine Learning Simulations for the Design of Lubricants



This month, Professor M. Clelia Righi, a full professor from the *University of Bologna*, joined our CMCC Mechanochemistry Discussions Seminar. She shared how her group uses ab initio and machine learning-informed molecular dynamics to study tribochemical reactions at sliding interfaces. Visit our channel to watch her seminar and learn how her work helps design more effective lubricants, including sustainable alternatives to petroleum-based oils.

We want to hear from you! Scan the QR code to take a short survey about our seminar series.



Scan the QR code to access the Spanish version!
¡Escanee el código QR para acceder a la versión en español!



Recent Presentations from CMCC Faculty



Dr. Alison Altman, professor at *Texas A&M University*, presented "Developing a Chemical Intuition for Orbital Specific Control in Lanthanide Complexes," at the Rare Earth Research Conference in Lemont, Illinois.



Dr. Andrew Rappe, professor at the *University of Pennsylvania*, presented "Stretching the Limits of Surface Reactivity: Mechanochemistry and Topological Catalysis," at the Italian Institute of Technology in Genoa, Italy.



Dr. Isaiah Speight, professor at *William & Mary*, presented "3D Printing and 3D Frameworks: Mechanochemical Approaches to New MOFs and Sustainable Synthesis," at the Canadian Society of Chemistry Conference in Ottawa, Ontario, Canada.

Recent Conference Presentations from CMCC Members at Texas A&M University



Dr. Mark Boyer, a postdoc in the Tabor group, presented "Hunting for Spectroscopically Observable Anharmonic Effects in Mechanochemically Accelerated Reactions," at the International Symposium for Molecular Spectroscopy in Urbana, Illinois.



Dr. Emmanuel Nwoye, a postdoc in the Batteas and Felts group, presented the "Experimental Quantification of Impact Force and Energy for Mechanical Activation in Vibratory Ball Mills," at the 29th Green Chemistry & Engineering Conference in Pittsburgh, Pennsylvania.



EJ Broker, a graduate student in the Batteas group, presented "Employing Atomic Force Microscopy as a Tool for the Mechanochemical Patterning of Graphene," at the SPMConnect at the TechConnect World Innovation Conference in Austin, Texas.



Katie Floyd, a graduate student in the Batteas group, presented "Systematic Examination of the Role of Silica Additive Properties on the Kinetics of the Mechanochemical Tolbutamide Synthesis," at the 29th Green Chemistry & Engineering Conference in Pittsburgh, Pennsylvania.

Welcome Our Newest Members at the CMCC!



Samuel Gunter
Graduate Student in the
Felts group at *Texas A&M University*



Rodney Amankwah
Undergraduate Student in the
Speight group at *William & Mary*



Evie Scally
Undergraduate Student in the
Speight group at *William & Mary*