## NSF Center for the Mechanical Control of Chemistry February 2025

Dr. Speight Featured on Concentrating on Chromatography Podcast



Dr. Isaiah Speight, an assistant professor at William & Mary, recently joined the Concentrating on Chromatography podcast to discuss innovative synthesis techniques. He discussed his research work on reducing waste and improving efficiency through advanced purification methods, including HPLC and flash chromatography for reaction monitoring. Dr. Speight also highlighted efforts to minimize solvent waste and introduced some of his ongoing and future projects. These include the development of 3D printed reaction vessels and mechanical catalysis, a process that uses physical forces instead of harsh chemicals to create safer chemical synthesis methods.

Scan the QR code to watch the full episode!

## Catch Our 2024 REU Cohort in Action at the ACS Meeting in March!

#### Poster Presentations: March 24, 2025, 12:00 - 2:00 PM Location: Hall B2/C

#### • Ethan W. Clare:

Force induced electron-rich lanthanide complexes from trivalent precursors and alkali metals

#### • Vanessa Dunu & Amelia Klaus:

Printing possibilities: The approach of additive manufacturing for accessible and sustainable chemistry

#### Andrew Foster:

When less isn't more: Isolation of mechanochemically generated calcium-based Grignard reagents

#### Maximillian Hauschildt:

Thermodynamic analysis of the solid-state mechanochemical MnBi-MnBi<sub>2</sub> reaction

#### • Angela Liu:

Mechanochemical approach to L-hexose synthesis

#### • Ryan O'Shea

Toward Lanthanide-based 2D Magnetic Materials

#### Robert Suber:

Understanding stereoselectivity of Heck cross-coupling reactions under mechanochemical conditions

#### Daniel Williams:

Building a mechanochemical reaction database for collaborative research and design

Oral Presentation: March 26, 2025, 10:55 - 11:15 AM Location: Hall G/H, Room 9

• Ryan O'Shea:

Quantum phenomena in lanthanide-based layered materials



### Illuminating Interfacial Mechanics: Utilizing Mechanophores to Quantify Stress in Polymer Composites

Learn how interfaces control polymer properties in this month's CMCC Mechanochemistry Discussion seminar! On February 20, Dr. Chelsea Davis will present new tools for measuring the micromechanical behavior of polymer surfaces and interfaces. By using fluorescent mechanophores and confocal imaging, her research reveals stress distribution and interfacial strength in composites, offering key insights into material performance and failure.

Watch here and join us every third . Thursday of the month!





Alumni Spotlight: Dr. Sayan Banerjee



Dr. Sayan Banerjee is currently a postdoctoral at the California Institute of researcher Technology, where he works with Dr. Jonas Peters on electrocatalytic processes. His current research focuses on developing mechanistic frameworks for N<sub>2</sub>-to-NH<sub>3</sub> conversion, combining computational and experimental approaches. In Fall 2025, Dr. Banerjee will join the University of Tennessee, Knoxville as an Assistant Professor in the Department of Chemistry. Dr. Banerjee completed his Ph.D. at the University of Pennsylvania under the mentorship of Dr. Andrew Rappe, where he explored catalytic reactions and material design. The research in the Banerjee lab will focus on creating predictive energy-efficient technologies, models for advancing electrochemistry, catalysis, and sustainability.

# Advancing Mechanochemistry: Mechanochemistry Reaction Database Reaction



The NSF Center for the Mechanical Control of Chemistry (CMCC) has developed and launched the Mechanochemical Reactions Database (MRD), a collaborative effort by Dr. Daniel Tabor, Dr. Adam Braunschweig, Dr. James Batteas, Dr. Jonathan Felts, Dr. Tim Hanusa, and Dr. Mateusz Marianski. This database builds upon the open-source Open Reaction Database from the NSF Center for Computer-Aided Synthesis (C-CAS). A key challenge in mechanochemistry is scaling reactions from the atomic level to the macroscale while maintaining high predictability in yield and selectivity. However, like many chemical synthesis processes, mechanochemical reactions are influenced by various factors-such as differences in instruments and materials—leading to significant variability in results. The MRD provides a centralized platform for the mechanochemistry community to share reaction conditions and outcomes. By compiling data, the database will help advance machine learning tools, enabling more accurate predictions of mechanochemical reactions.

Scan the QR code or visit our website to access the MRD!

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