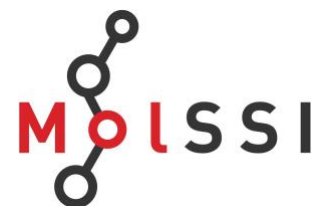


20th MERCURY Conference on Computational Chemistry

Furman University

July 18 – 22, 2022

Greenville, SC



Welcome

Welcome to the 20th MERCURY Conference on Computational Chemistry! We are delighted to see so many of you here again. We have assembled an outstanding group of speakers and about 70 students will present posters of their research. Undergraduate students will have opportunities to learn about the breadth of research being conducted in the field, and students and faculty will be able to meet and discuss their work with other computational chemists. Furthermore, this year's Molecular Sciences Software Institute (MoSSI) workshop will give participants opportunities to write programs and work in a collaborative software development environment.

This conference is organized by the MERCURY (**M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate **C**omputational **C**hemist**R****Y**) group, an organization of investigators at predominately undergraduate institutions, funded by a National Science Foundation NSF-MRI grant. NSF and Furman University provided most of the support for this conference. The Molecular Sciences Software Institute (MoSSI) also contributed to making this year's conference a success.

After the conference, we will ask for your feedback via a web survey to help us improve the conference. We hope you will take the time to respond to the survey. If you have any questions or problems, please contact:

Important Contacts

Tony McGuirt, Furman University, Facilities Services Administrator – 864.901.3727

Sabrina Pettaway, Furman University, Admin. Assistant – 864.772.9132

Lisa Green, Furman University Auxiliary Services - 864.608.9178

Paul Nerenberg, California State University, LA, MoSSI – 617.529.3930

George C. Shields, MERCURY Consortium, Founding Member – 864.907.8999

MERCURY Consortium Members

2001

George C. Shields
Maria Gomez
Carol Parish

Furman University
Mount Holyoke College
University of Richmond

2008

Maria Nagan
Tricia Shepherd
Kelling Donald
Adam Van Wynsberghe

Stony Brook
Franklin and Marshall College
University of Richmond
Hamilton College

2012

Kelly Anderson
Sudeep Bhattacharyay
Daqing Gao
Aimée Tomlinson
Jim Phillips

Roanoke College
University of Wisconsin - Eau Claire
Central State University
University of North Georgia
University of Wisconsin - Eau Claire

2016

Mychel Varner
Chrystal Bruce
Bill Miller
Joshua Schrier
Ashley Ringer McDonald
Dmytro Kosenkov
Juan Navea
Isaiah Sumner
George Barnes

Iona College
John Carroll University
Truman State University
Fordham University
Cal Poly San Luis Obispo
Monmouth University
Skidmore College
James Madison University
Siena College

2018

Heidi Hendrickson
He Kedan
Aurelia Ball
Joseph Baker

Lafayette College
Eastern Connecticut State University
Skidmore College
The College of New Jersey

2019

Sarah Arradondo
Robert Berger
Clyde Daly
Casey Londergan
Tyler Luchko
Lindsey Madison
Simba Nkomo
Paul Nerenberg
Anton Oliynyk
Caitlin Scott
Olaseni Sode
Patricia Soto

Washington College
Western Washington University
Haverford College
Haverford College
California State University Northridge
Colby College
Oxford College
California State University LA
Manhattan College
Hendrix College
California State University LA
Creighton University

2022

Nicole Adelstein
Petia Bobadova
Haoyuan Chen
Juan Duchimaza Heredia
Maduka Ogba
Luiz Oliverira
Jeff Schriber
Dom Sirianni
Frank Vazquez

San Francisco State University
Appalachian State University
UT RioGrande Valley
Emmanuel College Boston
Chapman University
Mount Vernon Nazarene University
Iona College
Daemen College
St. John's University

Conference Program

Monday, July 18, 2022

3:00 - 8:00 pm MoISSI: Check-in
Location: Judson Hall

6:00 - 7:00 pm MoISSI: Dinner
Location: Dining Hall

Tuesday, July 19, 2022

7:00 - 8:30 am MoISSI: Breakfast
Location: Dining Hall

9:30 am - 12:15 pm MoISSI: Workshop Day 1, AM Session
Welcome, Intro. To Electronic Structure Calculations, Setting Up a conda Environment, Geometry Optimization
Location: Patrick Lecture Hall, Townes Science Center

12:15 - 1:30 pm MoISSI: Lunch
Location: Dining Hall

1:30 - 3:30 pm MoISSI: Workshop Day 1, PM Session #1
Torsion Potential Energy Scan, Intermolecular Potential Energy Scan
Location: Patrick Lecture Hall, Townes Science Center

3:30 - 4:00 pm Coffee break
Location: Outside of Patrick Lecture Hall

4:00 - 5:15 pm MoISSI: Workshop Day 1, PM Session #2
Vibrational Frequencies and Basis Set Convergence
Location: Patrick Lecture Hall, Townes Science Center

6:00 - 7:00 pm MoISSI: Dinner
Location: Dining Hall

Wednesday, July 20, 2022

7:00 - 8:30 am MoISSI: Breakfast
Location: Dining Hall

9:00 - 10:45 am MoISSI: Workshop Day 2, AM Session #1
Redox Calculations
Location: Patrick Lecture Hall, Townes Science Center

10:45 - 11:00 am	Coffee break Location: Outside of Patrick Lecture Hall
11:00 - 12:15 pm	MolSSI: Workshop Day 2, AM Session #2 <i>Git and GitHub</i> Location: Patrick Lecture Hall, Townes Science Center
12:15 - 1:30 pm	MolSSI: Lunch Location: Dining Hall
1:30 - 3:45 pm	MolSSI: Workshop Day 2, PM Session <i>Putting It Together: A Capstone Activity, Wrap-up</i> Location: Patrick Lecture Hall, Townes Science Center
2:00 - 6:00 pm	General Check-In and Registration Location: Judson Hall
6:00 - 8:00 pm	Picnic Location: The Paddock (lower level of the Trone Student Center)
8:00 pm - 12:00 am	Social Gathering Location: The Paddock

Thursday, July 21, 2022

8:30 - 8:40 am	Opening Remarks Location: Burgiss Theatre, Trone Student Center
8:40 - 9:40 am	Henry F. Schaefer, University of Georgia Location: Burgiss Theatre
9:40 - 10:40 am	Brenda Rubenstein, Brown University Location: Burgiss Theatre
10:40 - 11:10 am	Coffee Break Location: Outside Burgiss Theatre (Trone Student Center 202)
11:10 am - 12:10 pm	Mai-Anh Ha, National Renewable Energy Lab Location: Burgiss Theatre
12:10 - 12:30 pm	Conference Picture Location: Dining Hall Front Steps
12:30 - 1:30 pm	Lunch Location: Dining Hall

1:30 - 3:00 pm Students' 1-Minute Talks
Location: Burgiss Theatre

3:00 - 4:15 pm Poster Session I: P1 – P33
Location: Watkins Room

4:15 - 5:30 pm Poster Session II: P34 – P66
Location: Watkins Room

5:30 - 7:00 pm Dinner
Location: Dining Hall

8:00 pm - 12:00 am Social Gathering
Location: The Paddock

Friday, July 22, 2022

7:00 - 8:30 am Breakfast
Location: Dining Hall

9:00 - 10:00 am Lela Vukovic, University of Texas at El Paso
Location: Burgiss Theatre

10:00 - 11:00 am Rigoberto Hernandez, Johns Hopkins University
Location: Burgiss Theatre

11:00 - 11:30 am Coffee Break
Location: Outside Burgiss Theatre (Trone Student Center 202)

11:30 am - 12:30 pm Mary Jo Ondrechen, Northeastern University-
Location: Burgiss Theatre

12:30 - 1:30 pm Lunch
Location: Dining Hall

12:20 - 2:30 pm Conference Checkout
Location: Judson Hall