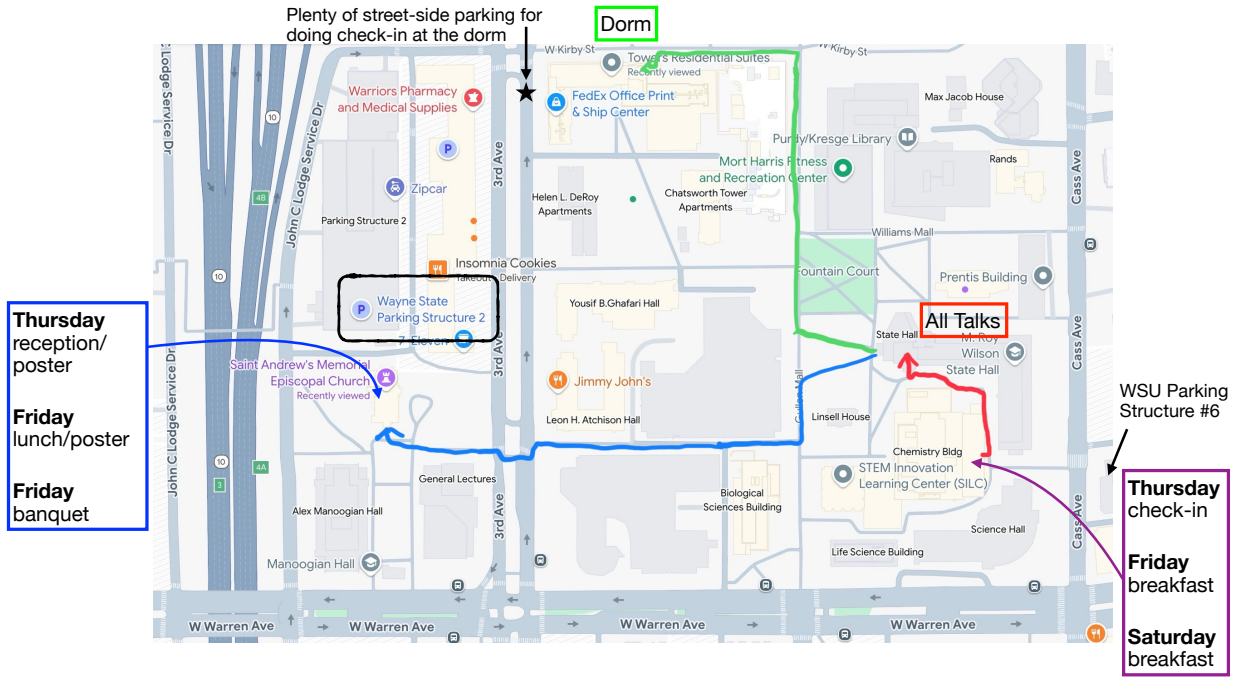
# 55th Midwest Theoretical Chemistry Conference (MWTCC55)
# May 29-31, 2025 • Wayne State University, Detroit, MI




| | Thursday 5/29 | Friday 5/30 | Saturday 5/31 |
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| **Atrium in the Chemistry Building** | 1pm: Check-in | 7am: Breakfast<br>Two coffee breaks | 7am: Breakfast<br>One coffee break |
| **State Hall 1101*** | Talks | Talks | Talks |
| **St. Andrew's Church** | 6pm: Reception + poster | 12pm: Lunch + poster<br>6:30pm: Banquet | |

*Access Room 1101 State Hall: enter at the red arrow, turn left immediately, and you will see the room on the right.

***Organizers:*** Zhenfei Liu, Alice Walker, Berny Schlegel, Vladimir Chernyak, and Matt Allen

<u>Thursday, May 29 afternoon</u> (Presider: Zhenfei Liu)

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| 1:00 – 3:45 | Check-in [Chemistry] |
| 4:00 – 4:10 | Welcome and Opening Remarks |
| 4:10 – 4:45 | **KEYNOTE: Paul Zimmerman** (Michigan)<br>*Strengthening the Ties between Wave Function Theory and Density Functional Theory* |
| 4:45 – 5:10 | **INVITED: Alex Dickson** (Michigan State)<br>*Undirected Exploration and Screening of Binding Pockets with Flexible Topology* |
| 5:10 – 5:35 | **Alexander Rusakov** (Oakland)<br>*Theory-Driven Investigation into the Chemistry of Superheavy Elements and Their Homologs* |
| 5:35 – 5:50 | **Neha Rani** (Wayne State)<br>*Mechanistic Studies and Theoretical Insights: From Water Splitting with Quinoline-Cobalt Complexes to the Surprising Thiol Selectivity in Furanosylations* |
| 6:00 – 8:00 | Reception and Poster Session #1 [St. Andrew's Church] |

Friday, May 30 morning (Presider: Berny Schlegel)

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| 7:00 – 7:45 | Breakfast [Chemistry] |
| 8:00 – 8:35 | **KEYNOTE: Angela Wilson** (Michigan State)<br>*Quantum Mechanical Perspectives on Transition Metal and Heavy Element Species* |
| 8:35 – 9:00 | **INVITED: Yang Yang** (Wisconsin)<br>*Constrained Nuclear-Electronic Orbital Framework for Modeling Hydrogen Chemistry* |
| 9:00 – 9:25 | **Lee Thompson** (Louisville)<br>*Beyond Orthogonality: Nonadiabatic Chemistry through a Nonorthogonal Lens* |
| 9:25 – 9:40 | **George Elliott** (Iowa State)<br>*Recent Advancements in QM-EFP* |
| 9:40 – 9:55 | **Donna Odhiambo** (Ohio State)<br>*Multireference Algebraic Diagrammatic Construction Theory for Core-Excited States* |
| 9:55 – 10:25 | Intermission |
| 10:25 – 10:50 | **INVITED: Roel Tempelaar** (Northwestern)<br>*Mixed Quantum–Classical Modeling of Quantum Materials* |
| 10:50 – 11:15 | **Kevin Carter-Fenk** (Pittsburgh)<br>*Single-Reference Theories for Calculating Electronic Spectra of Strongly-Correlated Systems* |
| 11:15 – 11:30 | **Anna Schouten** (Chicago)<br>*Bootstrapping the Electronic Structure of Quantum Materials* |
| 11:30 – 11:45 | **Xiao Zhu** (Indiana)<br>*A Large Language Model-Type Architecture for High-Dimensional Molecular Potential Energy Surfaces* |
| 11:45 – 12:00 | **Taylor Parsons** (Kansas)<br>*Simulating Absorption Spectra Using EOM-CCSD with a Polarizable Force Field* |
| 12:00 – 2:00 | Lunch and Poster Session #2 [St. Andrew's Church] |

Friday, May 30 afternoon (Presider: Zhenfei Liu)

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| 2:30 – 2:55 | **INVITED: Yuan Ping** (Wisconsin)<br>*Spin Relaxation and Chiral-Optical Properties of Solids from First-principles Density-Matrix Dynamics* |
| 2:55 – 3:20 | **INVITED: Noa Marom** (Carnegie Mellon)<br>*Computational Discovery of New Materials for Singlet Fission in the Solid State* |
| 3:20 – 3:45 | **Hsing-Ta Chen** (Notre Dame)<br>*Collective Optical Response and Local Molecular Dynamics in Disordered Light-Matter Systems* |
| 3:45 – 4:00 | **Gaurav Harsha** (Michigan)<br>*Exploring the Phase Diagram of α-Sn Using Self-Consistent GW* |
| 4:00 – 4:15 | **Bhavnesh Jangid** (Chicago)<br>*Multi-Reference Methods for Accurate Band Structure Calculations in Strongly Correlated Crystalline Periodic Systems* |
| 4:15 – 4:45 | Intermission |
| 4:45 – 5:10 | **INVITED: Wenzhe (Victor) Yu** (Argonne)<br>*Advancing Large-Scale Excited-State Materials Simulations for Quantum Technologies* |
| 5:10 – 5:35 | **Andrew Sand** (Butler)<br>*Characterization of Electron Transport in Molecular Devices and Wires Using Active Space Methods* |

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| 5:35 – 5:50 | **Varsha Kumari** (Indiana)<br>*Symmetry and Chemical Stability of 2D $M_3X_8$ (M = Nb, X= Cl, Br, I) and Other Ionic Kagome Materials* |
| 5:50 – 6:05 | **Gyanu Kafle** (Wayne State)<br>*Unveiling Phonon-Assisted Optical Properties of $MoS_2$ Bilayers* |
| 6:05 – 6:15 | Poster Award |
| 6:30 – 8:30 | Banquet [St. Andrew's Church]<br>*After-Dinner Talk:* **Krishnan Raghavachari** (Indiana) & **Berny Schlegel** (Wayne State) |

Saturday, May 31 morning (Presider: Alice Walker)

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| 7:00 – 7:45 | Breakfast [Chemistry] |
| 8:00 – 8:10 | Presentation from organizers of MWTCC56 in 2026 |
| 8:10 – 8:45 | **KEYNOTE: Krishnan Raghavachari** (Indiana)<br>*Coupled Cluster Accuracy at DFT Cost: Interpretable Graph-Network Based Machine Learning Models via Molecular Fragmentation* |
| 8:45 – 9:10 | **INVITED: Ming Chen** (Purdue)<br>*Guiding Deep-Learning Model to Explore "Constraint" Protein Conformational Ensemble* |
| 9:10 – 9:25 | **Eleanor Vandel** (U of Illinois Urbana-Champaign)<br>*Impacts of Static Disorder on the Quantum Dynamics of Dissipative Two-Level Systems* |
| 9:25 – 9:40 | **Ericka Miller** (Notre Dame)<br>*Product Directed Exploration of Chemical Reaction Networks* |
| 9:40 – 9:55 | **Paige Bowling** (Michigan)<br>*Efficient Exploration of Protein-Ligand Alchemical Landscapes using Seeded Multisite Lambda Dynamics* |
| 9:55 – 10:25 | Intermission |
| 10:25 – 10:50 | **INVITED: Jan-Niklas (Nik) Boyn** (Minnesota)<br>*Toward a Solution to the Static Correlation Error with a Hybrid Density Functional 1-RDMFT Framework* |
| 10:50 – 11:05 | **Prince Kwao** (North Dakota)<br>*On Generalized Eigenvalue Problem in Quantum Algorithms for Excited States* |
| 11:05 – 11:20 | **Siqin Cao** (Wisconsin)<br>*Memory Kernels of the Protein Dynamics: Developing Non-Markovian Models for Large Biomolecules* |
| 11:20 – 11:35 | **Anton Perera** (Case Western Reserve)<br>*Decoding The Structural Dynamics of Dye-Modified DNA Nanowires Using Classical Simulations* |
| 11:35 – 11:50 | **Vishaka Pathiranage** (Wayne State)<br>*Designing Fluorescent Protein-Based Anion Sensors for Live-Cell Imaging: A Computational Perspective* |
| 11:50 – 12:00 | Five-Minute, Five-Question Survey; Concluding Remarks |

WAYNE STATE UNIVERSITY Department of Chemistry

WAYNE STATE College of Liberal Arts and Sciences

CO MP American Chemical Society's Division of Computers in Chemistry

The Physical Chemistry Division of the American Chemical Society

APL Computational Physics

Gaussian, Inc.