

ISMPC 2024 Schedule

June 12-14, 2024

Pennsylvania State University

Registration, breakfast, lunch, and the poster session will be held on the third floor of the **Benkovic Building, Room 301A**

Oral sessions will be held in the **Thomas Building, Room 102**

Maps available at: https://www.k-state.edu/chem/conferences/ismpc_2024/attendees/transportation/transportation.html

Zoom link: <https://psu.zoom.us/j/95818611106>

Wednesday, June 12

7:30 a.m. Breakfast/Registration (Benkovic Building)

8:10 a.m. Transition to Thomas Building

8:20 a.m. Welcome

Session 1: Electronic Structure and Structure-Property Relationships

Presider: Ken Knappenberger (Penn State)

8:30 a.m. Tatsuya Tsukuda (The University of Tokyo): "Electronic Structures and Optical Properties of Chemically-modified Gold Superatoms"

9:00 a.m. Hannu Häkkinen (University of Jyväskylä): "Prospects and Challenges for Computer Simulations of Monolayer-protected Metal Clusters"

9:30 a.m. Sukhendu Mandal (Indian Institute of Science Education and Research Thiruvananthapuram): "Structure-Property Correlation in Atomically Precise Silver and Copper Nanoclusters"

10:00 a.m. Break

Session 2: Advances in Synthesis and Structural Control and Characterization

Presider: Rongchao Jin (Carnegie Mellon)

10:30 a.m. Thalappil Pradeep (Indian Institute of Technology Madras): "Carboranethiols: Versatile Ligand Platform for Atomically Precise Clusters"

11:00 a.m. Anindita Das (Southern Methodist University): "Atomically Precise Metal Nanochemistry with Stibine-Based Ligands"

11:30 a.m. Kevin Stampelcoskie, Queen's University, "Photochemical Synthesis, Purification, and Characterization of Thiol and Carbene Stabilized Gold Nanoclusters"

12:00 p.m. Vivek Yadav (Indian Institute of Technology Madras): "Optical Modulation by Site-specific Atomic Doping in M_{17} Nanoclusters: The Case of Ag_{17} , $AuAg_{16}$, Cu_4Ag_{13} and $AuCu_4Ag_{12}$ "

12:15 p.m. Subarna Maity (The University of Tokyo): "Surface Plasmon Resonance of Gold Ultrathin Nanorod with Few-atomic Silver Shell"

12:30 p.m. Lunch (Benkovic Building)

Session 3: Applications in Biology/Bioimaging

Presider: Ben Lear (Penn State)

- 1:30 p.m. Jie Zheng (The University of Texas at Dallas): "Transport and Interactions of Gold Nanoparticles in the Kidneys"
- 2:00 p.m. Stacy Copp (University of California, Irvine): "DNA Scaffolds for Atomically Precise Silver Nanoclusters"
- 2:30 p.m. María Francisca Matus (University of Jyväskylä): "Computational Tuning of Gold Nanoclusters for Targeted Cancer Therapy"
- 3:00 p.m. Viveka Kulkarni (Queen's University): "Ligand-Engineering of NHC-Protected Au₁₃ Nanoclusters for Efficient Generation of Reactive Oxygen Species"
- 3:15 p.m. Yitong Wang (Carnegie Mellon University): "Tailing Ligand and Kernel Structure Enhances NIR Photoluminescence of Atomically Precise Gold Nanoclusters"

3:30 p.m. Break

4:00 – 6:00 p.m. Poster Session (Benkovic Building)

Thursday, June 13

7:30 a.m. Breakfast/Registration (Benkovic Building)

Session 4: Exciting Applications

Presider: Rongchao Jin (Carnegie Mellon)

- 8:00 a.m. Yan Zhu (Nanjing University): "Catalysis Application of Atomically Precise Metal Clusters"
- 8:30 a.m. Meng Zhou (University of Science and Technology of China): "Triplet Excited State Dynamics of Metal Nanoclusters"
- 9:00 a.m. George Schatz (Northwestern University): "Electronic Structure Studies of Plasmonic Cluster Properties: Pressure Effects and Photocatalysis"
- 9:30 a.m. Noelia Barrabés (TU Wien): "Role of Ligands in Shaping the Properties and Reactivity of Gold Nanoclusters"

10:00 a.m. Break

Session 5: Advances in Theoretical Approaches

Presider: Christine Aikens (Kansas State)

- 10:30 a.m. De-en Jiang (Vanderbilt University): "From Supervised Learning to Generative Models in Atomically Precise Nanochemistry"
- 11:00 a.m. Andre Clayborne (George Mason University): "From Density Functional Theory to Quantum Information Science: Investigations of Superatoms using Computational Approaches"
- 11:30 a.m. Lasse Jensen (Penn State University): "Cluster Models in Surface-Enhanced Raman Scattering"
- 12:00 p.m. Alfredo Tlahuice (Universidad Autónoma de Nuevo León): "New 5-steps Algorithm to Speed up Structural Prediction of Thiolated Gold Clusters"
- 12:15 p.m. Maryam Sabooni Asre Hazer (University of Jyväskylä): "Theoretical Study on Metal-ligand Bond in Complexes and Clusters of Cu, Ag, and Au, with Thiolates, Phosphines, Alkynyls and N-Heterocyclic Carbenes"

12:30 p.m. Lunch (Benkovic Building)

Session 6: Physical Properties of Nanoclusters

Presider: Ben Lear (Penn State)

- 1:30 p.m. Joanna Olesiak-Banska (Wroclaw University of Science and Technology): "Ultra-small Noble Metal Nanoclusters as Markers in One-photon and Two-photon Fluorescence Microscopy"
- 2:00 p.m. Daniel Heintzelman (Penn State University): "Influence of Cluster-Solvent Hydrogen Bonding on MPC Optical Properties"
- 2:15 p.m. Haru Hirai (The University of Tokyo): "Photoluminescence and Photoredox Catalysis of Ligand-Protected MAu₁₂ Clusters: Effects of Dopant M and Halide Ligands"

- 2:30 p.m. Alessandro Fortunelli (Council for National Research of Italy (CNR)): "Experimentally-Validated Computational Prediction of the Chiro-Optical Response of Metallic Clusters and other Nanostructures"
- 2:45 p.m. Li-Juan Liu (The University of Hong Kong): "Atomically Precise Gold Nanoclusters at the Molecular-to-metallic Transition with Intrinsic Chirality from Surface Layers"
- 3:00 p.m. Subhradip Kundu (University of Geneva): "NMR Spectroscopy of Ag₂₉ Nanocluster"
- 3:15 p.m. Kristen Aviles (Penn State University): "Chain Length Control Over the Electronic Structure of Alkanethiolate Stabilized Palladium Nanoparticles Revealed by Conduction Electron Spin Resonance and Evans Method"
- 3:30 p.m. *Break*

Session 7: Synthesis: Understanding and Assemblies

Presider: Chris Ackerson (Colorado State)

- 4:00 p.m. Christopher Johnson (Stony Brook University): "Towards an Intuitive Framework to Explain Synthetic Control of Electronic Structure and Surface Chemistry of Metal Nanoclusters by Doping and Ligand Derivatization"
- 4:30 p.m. Thomas Bürgi (University of Geneva): "Encapsulation of Gold Clusters into Molecular Cavities"
- 5:00 p.m. Nonappa Nonappa (Tampere University): "Nanoconfinement Effect in Gold Superclusters"
- 5:30 p.m. Robert Whetten (Northern Arizona University): "PEGylation Revolution in NanoMedicine ... and in MPCs"

Friday, June 14

7:30 a.m. Breakfast/Registration (Benkovic Building)

Session 8: Royce Murray Memorial Session

Presider: Mary Beth Williams (Penn State)

8:00 a.m. Mary Beth Williams (Penn State University)

8:10 a.m. Dongil Lee (Yonsei University): "Rationally Designed Metal Nanoclusters for Electrocatalytic CO₂ Reduction"

8:40 a.m. Shaowei Chen (University of California, Santa Cruz): "Interfacial Chemistry of Organically Capped Nanoparticles"

9:10 a.m. Gangli Wang (Georgia State University): "Kinetics of Electrochemiluminescence from Metal Nanoclusters in Ratiometric Analysis and Electrocatalysis"

9:40 a.m. Rajesh Sardar (Indiana University – Purdue University Indianapolis): "Emerging optoelectronic properties of organo-metallic ligand-protected metal nanocrystals"

10:10 a.m. Announcement of next ISMPC; Poster Award presentation

10:30 a.m. Break

Session 9: Applications in Catalysis and Electrochemistry

Presider: Chris Ackerson (Colorado State)

11:00 a.m. Jian He (The University of Hong Kong): "Tuning the Structures and Catalytic Properties of Metal Nanoclusters via Ligand Engineering"

11:30 a.m. Robert Scott (University of Saskatchewan): "Total Scattering to the Rescue: Pair-Distribution Function Analysis of Supported Cluster Catalysts"

12:00 p.m. Marcus Tofanelli (Colorado State University): "Tuning Electron Transport Properties in MAu₂₅(PET)₁₈ Films: Effects of Superatomic Valence, Symmetry, and Counter Ion"

12:30 p.m. Lunch (Benkovic Building)