Graduate Research Symposium

GENERAL SCHEDULE

CHEMICAL DIVISION KEY

B Biological  P Physical  A Analytical
O Organic  M Materials  E Education
10:00 AM - KEYNOTE: Dr. Gabriel C.A. da Hora

Buruli Ulcer Disease: Tracking Toxin Pathogenicity with Enhanced Sampling Simulations

11:00 AM - 12:35 PM : Session 1, Tuesday

- **Myles Alan Lovasz** (Roberts) 11:00 AM - 11:25 AM
  Toward a modular synthesis of asymmetric and heteroatom-containing [2.2]paracyclopahnes

- **Mitchell Ellinwood** (Looper) 11:25 AM - 11:35 AM
  Development of a Semi-Synthetic Strategy to Inhibitors Against Rifampin Resistant Tuberculosis

- **Karsten Eastman** (Bandarian) 11:35 AM - 12:00 PM
  Mechanism and selectivity of peptide thioether crosslinks catalyzed by radical SAM enzymes

- **Austin LeSueur** (Sigman) 12:00 PM - 12:10 PM
  Identification of Active Chemical Space by Multi-Threshold Analysis

- **Kevin Beaver** (Minteer) 12:10 PM - 12:35 PM
  Nitric oxide signals for biofilm formation in mediated electron transfer microbial systems

**BREAK - 12:35 PM - 2:00 PM**

2:00 PM - 3:35 PM : Session 2, Tuesday

- **Ryan Spencer** (Steele) 2:00 PM - 2:25 PM
  Pushing Anharmonic Simulations to the Convergence Limit with Local Modes

- **Joshua Peterson** (Tang) 2:25 PM - 2:35 PM
  Energy transfer from CdS nanoparticles to Eu ligand complexes

- **Maryan Baraazande** (Tang) 2:35 PM - 2:45 PM
  Studying The CPL Activity of Chiral Si-QDs modified by Ligands with chiral helical frontier orbitals

- **Olavs Rāciņš** (Nagy) 3:00 PM - 3:10 PM
  Coupling Microdroplet-Based Derivatizations with Cyclic Ion Mobility Separations

- **Miharu Koh** (Harris, Minteer) 3:10 PM - 3:25 PM
  Confocal Raman Microscopy Analysis of pH-Induced Changes in Linear Poly(ethylenimine)
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GENERAL SCHEDULE
TBBC 4630

10:00 AM - KEYNOTE: Dr. Salvador Gutierrez Portocarrero

*Electrochemical Reactivity at the Organic-Water Interface*

11:00 AM - 12:35 PM: Session 1, Wednesday

- **E** Lorraine Laguerre Van Sickle (Frey) 11:00 AM - 11:25 AM
  Students' study habits as a predictor of performance in general chemistry
- **I** Jing Liu (Gao) 11:25 AM - 11:35 AM
  Aqueous Electrolytes Reinforced by Mg and Ca Ions for Highly Reversible Fe Metal Batteries
- **P** Asylbek (AJ) Zhanserkeev (Steele) 11:35 AM - 12:00 PM
  Enabling Anharmonic Spectroscopy Simulations via Improved Predictions of Mode Couplings
- **P** Kefu Wang (Tang) 12:00 PM - 12:10 PM
  Efficient Photon Upconversion Enabled by Strong Coupling Between Silicon QD and Organic Molecules
- **P** Samantha Walker (Armentrout) 12:10 PM - 12:35 PM
  Structural study of tripeptides with Zn & Cd dications in the gas phase using IRMPD and calculations

BREAK - 12:35 PM - 2:00 PM

2:00 PM - 3:10 PM: Session 2, Wednesday

- **O** Hanna Clements (Sigman) 2:00 PM - 2:25 PM
  An Interpretable and Predictive Enzyme Engineering Strategy
- **B** Delaney Beals (Puri) 2:25 PM - 2:35 PM
  Cultivation of methanotrophs in a spatially resolved model ecosystem
- **O** Zach Schwartz (Roberts) 2:35 PM - 3:00 PM
  Synthesis of [n]helicenes and polycyclic aromatics via deaminative contractions
- **O** Dionysius W. Copoulos (Looper) 3:00 PM - 3:10 PM
  The Synthesis and Biological Studies of a Novel Class of Naphthyridone Antibiotics
10:00 AM - KEYNOTE: Dr. Tsugunosuke Masubuchi
Understanding Sub-Nano Catalysis: Electrochemical Hydrogen Evolution at Size-Selected Pt Clusters

11:00 AM - 12:35 PM: Session 1, Thursday

- Nicholas Vitti (White) 11:00 AM - 11:25 AM
  Determination of the Critical Nucleus Size of Ag on Pt Nanoelectrodes
- Yunan Qin (Gao) 11:25 AM - 11:35 AM
  Exploring Carbonyl Chemistry in Non-aqueous Mg Flow Batteries
- Tim McFadden (Sigman, Minteer) 11:35 AM - 12:00 PM
  Uncovering subtle catalyst inhibitor relationships in Frontal Ring-Opening Metathesis Polymerization

BREAK - 12:35 PM - 2:00 PM

2:00 PM - 3:10 PM: Session 2, Thursday

- Paulina James (Tang) 12:00 PM - 12:10 PM
  Photon Upconversion in the Visible Wavelengths with ZnSe/InP/ZnS Nanocrystals
- Tsumugi Miyashita (Tang) 12:10 PM - 12:35 PM
  Investigating the triplet-triplet annihilation efficiency of diphenylanthracene isomers

- Hannah Burton (Swanson) 2:00 PM - 2:25 PM
  Multistate kinetic modeling explains disparate ion-flux with transmembrane potential
- Will Matthews (Grüenwald) 2:25 PM - 2:35 PM
  Predicting Crystallization from Solution Species
- Chelsea Valiton (Roberts) 2:35 PM - 3:00 PM
  One-pot deaminative contraction strategies to build polycyclic aromatic natural products
- Tingting Huang (Tang) 3:00 PM - 3:10 PM
  Bidirectional Triplet Exciton Transfer Between Silicon Nanocrystals and Perylene
The Development of the STEM Teaching Practices Faculty Inclusive Teaching Survey (ISTP FITS)

Networking Keynote talk with the Executive Director of Research and Infrastructure at Boston College, book author, and PhD biochemist.

2:00 PM - 5:00 PM Networking and Poster Session - Catered Henry Eyring Building Atrium

All presenters, judges, faculty, staff, and students are welcome at the Networking and Poster Session. Please enjoy the catered food and drinks. Thanks for everyone’s hard work this year!