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5th Annual CBE Graduate Research Symposium

Hosted By:
University of Notre Dame
Chemical and Biomolecular Engineering
Graduate Student Organization

September 19th 2019
Dahnke Ballroom
Duncan Student Center



Welcome

Welcome to the 5th Annual CBE Graduate Research Symposium! The goal of the CBEGSO Symposium is to provide a forum for CBE graduate students to present their research, network with professionals from both industry and academia, and develop their professional identity.

Over the course of the day, students will showcase research from a wide range of disciplines, including catalysis, energy and sustainability, nano-fluidics, micro-fluidics, simulation and theory, materials science, nanotechnology, and bioengineering.

The Symposium also features a keynote address and student speakers who won awards for Best Paper and Best Candidacy.

Poster awards will be announced at the end of the day. The four poster award winners will be given cash prizes and an opportunity to present their research at a department seminar.

As this event has continued to grow, so too has the impact on CBE graduate student professional development and sense of community.

Thank you for attending the CBEGSO Symposium!

Section for Notes

Event Schedule

9:30 A.M.

Setup/Registration

10:30 A.M.

Poster Session I – Odd Numbered Posters

11:30 A.M.

Lunch

12:30 P.M.

Keynote Address

1:45 P.M.

Poster Session II – Even Numbered Posters
and Group Photo

2:45 P.M.

Student Talks

3:45 P.M.

Closing Remarks and Poster Awards

Keynote Speaker



Yiannis Kaznessis is the founder of General Probiotics. He joined the company as Chief Executive Officer in 2017. Dr. Kaznessis is a Notre Dame Alumni, he received his PhD from the University of Notre Dame in 1999 in Chemical Engineering. He completed postdoctoral research at Pfizer Global R&D, and at the University of Michigan. Prior to starting his company, Dr. Kaznessis had an outstanding career in academia at the University of Minnesota. He joined the faculty in Chemical Engineering as an assistant professor in 2001 and was tenured and promoted to associate professor in 2007 and to full professor in 2011. He was a director of the Bioinformatics Summer Institute from 2004 to 2011. He held the position of Director of Graduate Studies from 2010 to 2017. He raised over \$7M in research funds and was the recipient of several honors and awards.

Symposium Organizing Board



Elvis Eugene



Matthew Sis



Jerry Crum



Justin Easa



Jessica Muhlenkamp



Derrick Poe



Galiya Magazova



Aubrey Jeffries



Dr. Jason Hicks

P. 36 Material Property Goals to Enable Continuous Diafiltration Membrane Cascades for Lithium-ion Battery Recycling
Elvis A. Eugene, William A. Phillip, Alexander W. Dowling

P. 37 Materials Characterization Facility
Ian Lightcap

Each poster is evaluated by two judges, on the basis of research rationale, experimental approach, use of data in support of conclusions, and overall presentation quality.

Recipients of the Best Poster Award receive a cash prize and the opportunity to present their work in a department seminar.

Student Speakers

Winner of Best Paper Award:



Vikramjit Singh Rathee is a recent Ph.D. graduate in Chemical & Biomolecular Engineering from Dr. Whitmer's group at University of Notre Dame. His doctoral research primarily focused on simulating behavior of pH-responsive polymers or weak polyelectrolytes and investigating their complexation process. He has also developed solid foundation in Machine Learning and has been involved with Neural Network, Convolutional Neural Network applications. His hobbies include playing sports, exercising, hiking and camping. More info about the work he has been involved with can be found on his website: vikramjitsinghrathee.com

Winner of Best Candidacy Award:

Hunter Ford is beginning his fourth year as a graduate student in Dr. Jennifer Schaefer's research group, and is researching the development of materials for use in rechargeable battery systems. Specifically, Hunter is interested in understanding means of manipulating transport properties within "beyond lithium-ion" energy systems with the use of functional polymers. Through understanding redox mechanisms and interactions between polymer and relevant electrochemical species, it is hoped that some of the fundamental challenges associated with next generation rechargeable batteries can be addressed. Hunter received his B.S. in chemical engineering and B.A. in chemistry from Hope College in Holland, Michigan. After graduating from Hope College Hunter worked in a product engineering role at Haworth Inc., a global office furniture manufacturing company, before attending Notre Dame in 2016.



- P. 29 Evolution of Surface and Bulk Carbonaceous Species Derived from Propylene
Justin Easa, Renxi Jin, Casey O'Brien

- P. 30 Kinetic Evaluation of Grafted, Single-Site Zr-H Catalysts for Ethylene Oligomerization
Galiya Magazova

- P. 31 Highly Selective Bimetallic Phosphides for Propane Dehydrogenation and the Role of P in Dehydrogenation
Jessica A. Muhlenkamp, Jeonghyun Ko, William F. Schneider, Jason C. Hicks

- P. 32 Selective Hydrogenation of Functionalized Carbonyls with Rh-Based Intermetallic Compounds
Aubrey Jeffries

- P. 33 A Study of Solvation Structure and Dynamic Properties of Ethaline and Glyceline via Molecular Dynamics
Derrick Poe, Yong Zhang, Edward Maginn

- P. 34 Selectivity in multiple guises: Microkinetic models of NH₃ catalytic oxidation
Hanyu Ma, William Schneider

- P. 35 Preparation and performance evaluation of single-ion (Na⁺/K⁺/Ca²⁺) conducting gel polymer electrolytes
Chuanchuan Cui, Hunter O. Ford, Jiacheng Liu, Peng He, Yubing Dou, Bumjun Park, Jennifer L. Schaefer

Poster Presentations

Odd numbered posters present session I, even numbered session II

- P. 22 Computational Interrogation of Single-Site, Oxide-Supported Group 4 Metal Hydrides for Ethylene Oligomerization
Neha Mehra, Galiya Magazova, Jason Hicks, William F. Schneider
- P. 23 Identification of a CD22 Receptor Binding Peptide and Evaluation of Its Potential Use for Acute Lymphoblastic Leukemia (ALL) Targeted Nanoparticle Drug Delivery System
Baksun Kim, Jaeho Shin, Tanyel Kiziltepe, Basar Bilgicer
- P. 24 Inhibition of Peanut Induced Mast Cell Degranulation by Designing Covalent Heterobivalent Inhibitors
Jaeho Shin, Peter Deak, Baksun Kim, Tanyel Kiziltepe, Basar Bilgicer
- P. 25 Liposomal Platform for Study and Optimization of Endosomal Escape
Franklin Mejia, Sabrina Khan, Basar Bilgicer
- P. 26 Targeted Liposomal DM1 Prodrug Formulation for Improved Anti-cancer Effect
Sabrina Khan, Franklin Mejia, Basar Bilgicer
- P. 27 Ni-MgO Stable and Active Catalysts for the Dry Reforming of Methane Prepared by Paper Assisted Combustion Synthesis
V. Danghyan, A. Muksayan, E. Wolf
- P. 28 The Effect of Ceramic Addition to Single Ion Conducting Polymers for Lithium Metal Batteries
Laura Merrill, Yiman Zhang, Hunter Ford, Jennifer Schaefer, Xi Chelsea Chen, Nancy Dudney

- P. 1 Portable immersed AC Electro spray (iACE) using glass micropipettes for conformal single cell hydrogel coating
Vivek Yadav, Zehao Pan
- P. 2 Highly Permeable and Selective Crosslinked Pentiptycene-based Polymer Membranes for Gas Separation
Si Li, Ruilan Guo
- P. 3 Integration of Molecular Simulations and Computer-Aided Design to Enable Novel Azeotropic Hydrofluorocarbon Separations
Bridgette Befort, Alexander Dowling, Edward Maginn
- P. 4 Intrinsically Microporous Pentiptycene-based Polymers for Enhanced Gas Separation Performance and Physical Aging Resistance
Tanner Corrado, Ruilan Guo
- P. 5 Gel Polymer Electrolytes for Metal-Sulfur Batteries: Effect of Crosslinker Repeat Chemistry on Polysulfide Interactions
Hunter Ford, Jizhou Jiang, Peng He, Jennifer Schaefer
- P. 6 Novel Elastic Response in Twist-bend Nematic Models
Jiale Shi, Hythem Sidky, Jonathan K. Whitmer
- P. 7 Non-solvating, side-chain polymer electrolytes as lithium single-ion conductors: synthesis and ion transport characterization
Jiacheng Liu, Bumjun Park, Sunil P. Upadhyay, Jennifer L. Schaefer

- P. 8 Understanding Binding Behavior in Host-Guest Systems Using Advanced Sampling Simulations
Anne C. Leonhard, Jonathan K. Whitmer
- P. 9 Obtaining a Mechanistic Understanding of Polyvinylamine-based Facilitated Transport Membranes for CO₂ Separation
Sarah Pate, Casey O'Brien
- P. 10 Kinetic modelling of catalytic reactions: Bridging the gap between mean-field and lattice-based Monte Carlo models
A. Bajpai, A. Goswami, W.F. Schneider
- P. 11 Identifying Immunodominant Epitopes of House Dust Mite Protein Der p 2
Jenna Sjoerdsma, Franklin Mejia Frias, Basar Bilgicer
- P. 12 Controlled post-assembly functionalization of nanoporous copolymer membranes that exhibit distinct multifunctionality
John R. Hoffman, Andrew Mikes, William A. Phillip
- P. 13 Microporous Polymeric Membrane for Gas Separations
Zihan Huang, Dr. Ruilan Guo
- P. 14 Interfacial Junctions Control Electrolyte Transport through Charge-Patterned Membranes
Feng Gao, William Phillip
- P. 15 Multiscale Modeling and Optimization of Solar Thermal Desalination Systems
Alejandro Garcadiago, Tengfei Luo, Alexander W. Dowling
- P. 16 Microkinetic Model Reduction and Oligomerization Reactor Optimization in CISTAR
Kanishka Ghosh, Alejandro Garcadiago, Alexander W. Dowling
- P. 17 High Free Volume Ionic Polymers for Fuel Cells and Water Desalination
Tao Wang
- P. 18 Investigation of the effects of copper nanoparticles on magnesium-sulfur battery performance: How practical is metallic copper addition?
Peng He, Hunter O. Ford, Laura C. Merrill, Jennifer L. Schaefer
- P. 19 Gaussian Process Regression and Stochastic Programming for Optimal Energy Market Participation
Xian Gao, Alexander W. Dowling
- P. 20 First-principles Analysis of Dicopper Species in Zeolites for O₂ Activation and Implications for Catalyst Optimization
Yujia Wang, Sichi Li, Tong Wu, William F. Schneider
- P. 21 Investigating CB/SERS Detector Capabilities as a Function of Cucurbit[7]uril Macrocycle Geometry on Nanoparticle Surface
Adam S. Braegelman, Leonhard Karger, Lei Zou, Jon P. Camden, Matthew J. Webber