UNIVERSITY OF NOTRE DAME
College of Engineering

Sept 2016 | 7

Chemical & Biomolecular Engineering

Graduate Student Organization

Presents

The 2nd Annual CBE

Graduate Research Symposium

Notre Dame Conference Center, McKenna Hall

Department of Chemical and Biomolecular Engineering
University of Notre Dame

Schedule

8:30 – 9:00 am	Refreshments & Pastries
9:00 – 10:25 am	Poster Session I
10:25 – 11:30 am	Session I
11:30 – 12:30 pm	Lunch
12:30 – 1:15 pm	Session II
1:15 – 1:30 pm	Break
1:30 – 2:30 pm	Alumni Panel
	Dr. Michael Penninger, *UOP Honeywell*
	Dr. Allison Cross, *Johnson Matthey*
2:30 – 2:45 pm	Break
2:45 – 3:45 pm	Session III
3:45 – 5:15 pm	Poster Session II
5:15 – 5:30 pm	Awards & Closing Remarks

Alumni Panelists

Dr. Allison Cross

Allison Cross received her B.S. in chemical engineering from Rose-Hulman Institute of Technology. She then received her M.S. and Ph.D. in chemical and biomolecular engineering from the University of Notre Dame with a thesis on heterogeneous catalysis for hydrogen production. Currently, she is working as a Catalyst Development Scientist at Johnson Matthey Process Technologies in Savannah, GA, doing product development of FCC additives.

Dr. Michael W. Penninger

Michael W. Penninger received the B.S. in chemical engineering from Western Michigan University, and the M.S. and Ph.D. in chemical and biomolecular engineering from the, University of Notre Dame, Notre Dame, Indiana. He held internships at Bosch, Pfizer, and General Motors. He is just finishing his first year as a Process Modeling Specialist with UOP Honeywell, Des Plaines, IL.

Student Oral Presentations

Session I 10:25 – 11:30am

10:30-10:45	Nonaqueous Microchip Electrophoresis for the Characterization of Lipid Biomarkers Erick Foster and Paul W. Bohn
10:45-11:00	Inhibitors for Allergic Reactions to Drugs and Other Small Molecules Peter E. Deak, Maura R. Vrabel, Vincenzo J. Pizzuti
11:00-11:15	Selectivity Enhancements in Microfluidic DNA Biosensors: Thermodynamics Versus Kinetics Steven Marczak, Satyajyoti Senapati, Hsueh-Chia Chang
11:15-11:30	Monte Carlo Simulations of Surfactants and the Air-Water Interface Brian Yoo, Yingxi Zhu, Edward J. Maginn

Session II 12:30 – 1:15pm

12:30-12:45	Semi-Interpenetrating Polymer Networks (SIPNs) for Synergistically Attractive CO2 Separation Performance and Improved Membrane Mechanical Robustness Gregory K. Kline and Ruilan Guo
12:45-1:00	Site-Specific Immobilization of Antibody on Gold Nanoparticle Surface for One-Step Diagnosis of Prostate Specific Antigen with Dynamic Light Scattering Nur Mustafaoglu, Jun Huang, and Basar Bilgicer
1:00-1:15	Discrete Fractional Component Monte Carlo Method for Phase Equilibrium Molecular Simulations Eliseo Marin-Rimoldi and Edward J. Maginn

Session III 2:45 – 3:45pm

2:45-3:00	Aging like a Fine Wine: A Study of Physical-Aging Enhanced Gas Transport in Triptycene-Based Polyimide Membranes Jennifer Wiegand and Ruilan Guo
3:00-3:15	Thermal Hazard Analysis and Chemical Incompatibility Test with Novel Custom High-Pressure Crucibles Made from Commonly Used Metals and Alloys Han Xia, Joan Brennecke
3:15-3:30	Catalysis in a Cage: Condition Dependent Speciation and Dynamics of Exchanged Cu Cations in Zeolites Christopher Paolucci, Hui Li, Fabio H. Ribeiro, Rajamani Gounder, and William F. Schneider
3:30-3:45	Morphogens regulate spatiotemporal-patterning of Ca(II) in a developing epithelium Pavel A. Brodskiy, Qinfeng Wu, Cody Narciso, Jeremiah J. Zartman

Poster Presentations

Poster Session I 9:00 – 10:30am

P.1	Probing Phosphonium Based AHA Ionic Liquids for CO_2 Capture Gabriela M. Avelar, Oscar Morales, Joan F. Brennecke
P.2	Fabrication of High-Performance Hollow Fiber Nanofiltration Membranes by Coating Uniform Nanoporous Films from Block Polymer Solutions Yizhou Zhang, Jessica L. Sargent, Bryan W. Boudouris, William A. Phillip
P.3	Membrane Separation of Biomolecules with Similar Size: A Coarse Grained Molecular Dynamics Simulation Study Yushan Zhang, Yong Zhang, Edward Maginn, Mark J. McCready
P.4	Morphogens regulate spatiotemporal-patterning of Ca(II) in a developing epithelium Pavel A. Brodskiy, Qinfeng Wu, Cody Narciso, Jeremiah J. Zartman
P.5	Probing the reactive NH_3 for fast SCR on H form SSZ13 from DFT and kinetics study Sichi Li , Yang Zheng , Feng Gao , Janos Szanyi , William F. Schneider
P.6	A Study of Polymer Backbone Flexibility in Triptycene-Based Copolyimides for Gas Separation Membranes Jennifer Wiegand and Ruilan Guo
P.7	Molybdenum-rich phosphide catalyst for biomass upgrading Yolanda Bonita, Jason C. Hicks
P.8	Inkjet Printing of Layer-by- Layer Assembled Charge Mosaic Membranes Feng Gao, Peng Gao, Aaron Hunter, Sherwood Benavides and William A. Phillip
P.9	Catalysis in a Cage: Condition Dependent Speciation and Dynamics of Exchanged Cu Cations in Zeolites Christopher Paolucci, Hui Li, Fabio H. Ribeiro, Rajamani Gounder, and William F. Schneider
P.10	Development of Descriptors to Enable Screening Calculations that Predict the Viscosity of Ionic Liquids Michael Humbert, Yong Zhang, and Edward J. Maginn

P.11	Site-Specific Immobilization of Antibody on Gold Nanoparticle Surface for One-Step Diagnosis of Prostate Specific Antigen with Dynamic Light Scattering Nur Mustafaoglu, Jun Huang, and Basar Bilgicer
P.12	Process Modeling For Separation of Aromatics From Aliphatics With Ionic Liquids Yuanyuan Lyu, Joan Brennecke, and Mark A. Stadtherr
P.13	Lithiated side-chain ionomers to enable studies on ion transport mechanisms in electrolytes Sunil Upadhyay and Jennifer L. Schaefer
P.14	Photonic and Quantum Interactions of Atomic-Scale Junctions Garrison Crouch, Paul W. Bohn
P.15	Nanoscale Thermal Hotspot by Focused Ohmic Heating Zehao Pan, Ceming Wang, Meng Li, and Hsueh-Chia Chang

Poster Session II 3:45 – 5:15 pm

P.16	A Molecular Dynamics Study of Actinide Nanoclusters Ken Newcomb, Edward J. Maginn
P.17	Intercellular Ca(ll) Transients Integrate Spatiotemporal Morphogenetic Patterning in the Drosophila Wing Imaginal Disc Qinfeng Wu, Pavel Brodskiy, Cody Narciso, and Jeremiah J. Zartman
P.18	pH-induced Hysteric Swelling of Charge Mosaic Membranes Prepared Using Layer-By-Layer Assembly Mark J. Summe, Sahadevan Rajesh, William A. Phillip
P.19	Inhibitors for Allergic Reactions to Drugs and Other Small Molecules Peter E. Deak, Maura R. Vrabel, Vincenzo J. Pizzuti, Basar Bilgicer
P.20	Structural Study of 1-Ethyl- 3-methylimidazolium with Aprotic Heterocyclic Anions Seungmin Oh, Oscar Morales, and Joan F. Brennecke

P.21	Iptycene Containing Polyimide/Modified ZIF-90 Mixed Matrix Membranes (MMMs) for Gas Separation Qinnan Zhang, Ruilan Guo
P.22	Ab-initio Molecular Dynamics for Copper Cation Mobility and Adsorption Free Energies in Zeolites Hui Li, Christopher Paolucci, William F. Schneider
P.23	Ionic Liquids as Extraction Solvents for Separating Aromatic and Aliphatic Compounds: Extraction and Solvent Regeneration Michael J. Lubben, Roberto I. Canales, and Joan F. Brennecke
P.24	A Molecular Understanding of the Cytotoxic Interactions of Ionic Liquids Towards a Lipid Biomembrane Brian Yoo, Yingxi Zhu, Edward J. Maginn
P.25	Nonaqueous Microchip Electrophoresis for the Characterization of Lipid Biomarkers Erick Foster and Paul W. Bohn
P.26	Nanoporous Block Polymer Thin Films Functionalized with Bio-Inspired Ligands for the Efficient Capture of Heavy Metal Ions from Water Jacob Weidman and William A. Phillip
P.27	Simultaneous Process and Material Design for Aprotic Heterocyclic Anion Ionic Liquid in Carbon Capture Systems Bo Hong, Joan F. Brennecke, and Mark A. Stadtherr
P.28	Interchange Reactions in the Ti-B- N System Joshua Pauls and Alexander S. Mukasyan
P.29	Low temperature, highly selective ketonization of acetic acid on well-defined, cerium incorporated MEL-type zeolites Nikhil S. Japtiwale, Nicholas D. McNamara, Kwan Lai Leon Tong, Jason C. Hicks
P.30	A Shear-CNT- DEP Nanoscale Electrokinetic Platform for UltraSensitive/Selective Protein Quantification with Tunable Dynamic Range: Overcoming Thermodynamic Limitations Diya Li, Ceming Wang, Satyajyoti Senapati and Hsueh-Chia Chang

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