

Ellis R. Crabtree

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EDUCATION

Johns Hopkins University – *Baltimore, Maryland* 05/2024 (expected)
Doctor of Philosophy (Ph.D.)
Department: Chemical and Biomolecular Engineering
Advisor: Professor Yannis G. Kevrekidis

Master of Science in Engineering (M.S.E.)
Department: Applied Mathematics and Statistics
Focus: Computational Mathematics

The University of Alabama – *Tuscaloosa, Alabama* 05/2019
Bachelor of Science in Chemical Engineering; *Magna Cum Laude, University Honors, ChBE Honors*
Major: Chemical Engineering
Minor: Mathematics

WORK EXPERIENCE

Johns Hopkins University – *Baltimore, Maryland* 08/2019 – Present
<https://jhu.edu>
PhD Candidate

- Using dimensionality reduction techniques and neural network based generative models for expediting sampling of dynamical systems
- Working with Sandia National Labs Combustion Research Facility to investigate machine learning and dimensionality reduction applications for uncertainty quantification
- Using generative models for separatrix identification in dynamical systems

Georgia-Pacific LLC – *Pennington, Alabama* 01/2016 – 08/2017
<https://gp.com> (3 Co-op rotations)
Process Engineering Co-op

- Worked in the process engineering and control group
- Ran and managed audits and trials around various process control systems
- Created new process control PIDs, guidelines, and limits to improve efficiency of black liquor solids flow from the pulp mill (estimated savings of \$1MM by time of departure)
- Updated current and created new Standard Operating Procedures for multiple efficiency tests

- Utilized molecular simulations to investigate the selective adsorption properties of ionic polyimides and ionic polyimide/ionic liquid composites
- Generated and analyzed molecular dynamics and structural analysis code
- Created 3D representations of molecular simulations utilizing design software and 3D printing

PROFICIENCIES

- | | |
|----------------------|---|
| • Skills | ML/Data Science, Monte Carlo Simulation, Molecular Dynamics |
| • Platforms | Windows, Linux, OS X |
| • Programming | FORTRAN, Python, Matlab, HTML, Java, SQL |
| • Important Packages | Pytorch, Tensorflow, Jax, OpenMM, GROMACS, CAD, Solidworks |
| • Language | English, Portuguese |

PUBLICATIONS AND PRESENTATIONS

Molecular Simulation of Ionic Polyimides and Composites with Ionic Liquids as Gas-Separation Membranes

Asghar Abedini, **Ellis Crabtree**, Jason E. Bara, C. Heath Turner

Langmuir 33 (42), **2017**, 11377-11389

DOI: 10.1021/acs.langmuir.7b01977

Molecular Analysis of Selective Gas Adsorption Within Composites of Ionic Polyimides and Ionic Liquids as Gas Separation Membranes

Asghar Abedini, **Ellis Crabtree**, Jason E. Bara, C. Heath Turner

Chemical Physics, Volume 516, **2019**, pp. 71-83

DOI: 10.1016/j.chemphys.2018.08.039

Molecular Transport Behavior of CO₂ in Ionic Polyimides and Ionic Liquid Composite Membrane Materials

Joanna Szala-Bilnik, Asghar Abedini, **Ellis Crabtree**, Jason E. Bara, C. Heath Turner

The Journal of Physical Chemistry B, **2019**, 123 (34), 7455-7463

DOI: 10.1021/acs.jpcb.9b05555

Solubility and Diffusivity of CO₂ in Ionic Polyimides with [C(CN)₃]^x[OAc]^{1-x} Anion Composition

Joanna Szala-Bilnik, **Ellis Crabtree**, Asghar Abedini, Jason E. Bara, C. Heath Turner

Computational Materials Science, Volume 174, **2020**, 109468, ISSN 0927-0256,

DOI: 10.1016/j.commatsci.2019.109468

GANs and Closures: Micro-Macro Consistency in Multiscale Modeling

Ellis Crabtree, Juan M. Bello-Rivas, Andrew L. Ferguson, Ioannis G. Kevrekidis

Multiscale Modeling and Simulation, 21 (3), **2023**, 1122-1146

Micro-Macro Consistency in Multiscale Modeling: Score-Based Model Assisted Sampling of Fast/Slow Dynamical Systems

Ellis Crabtree, Juan M. Bello-Rivas, Ioannis G. Kevrekidis

Arxiv preprint: 2312.05715, **2023**

2017 AIChE Annual Meeting – Minneapolis, Minnesota

October 2017

- Poster, “Molecular Simulation of Ionic Polyimides and Ionic Liquid Composites for Gas Separation”

2017 AIChE Annual Meeting – Minneapolis, Minnesota

October 2017

- Talk, “Gas Adsorption Behavior in Ionic Polyimide Composite Membranes”
- *Contributed – not main presenter*

2018 AIChE Annual Meeting – Pittsburgh, Pennsylvania

October 2018

- Talk, “Molecular Simulation of Ionic Polyimides and Ionic Liquid Composite Membranes for Gas Selectivity and Adsorption”
- *Contributed – not main presenter*

2021 AIChE Annual Meeting – Boston, Massachusetts

November 2021

- Talk, “Something Old, Something New: Generative Adversarial Approaches to Conditional Sampling in Complex System Simulations”

2023 SIAM Dynamical Systems conference – Portland, Oregon

May 2023

- Talk, “Generative Model Assisted Sampling of Multiscale Stochastic Dynamical Systems”

2023 AIChE Annual Meeting – Orlando, Florida

November 2023

- Talk, “Generative Model Assisted Sampling of Multiscale Stochastic Dynamical Systems”

HONORS AND AWARDS

DOE SCGSR Fellowship

- Fellowship to sponsor research at a DOE national lab

JHU ChemBE Department Graduate TA award

- Awarded to outstanding graduate student TAs in the ChemBE department at Johns Hopkins University

Randall Outstanding Undergraduate Research Award

- Recognizes outstanding undergraduate research conducted by students at the University of Alabama

University of Alabama Presidential Merit Scholarship

- Full academic scholarship provided by the University of Alabama