

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

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://jh.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

The University of Alabama – *Tuscaloosa, Alabama* 01/2015 – 07/2019
<https://ua.edu>
Undergraduate Research Assistant

- Utilize molecular simulations to investigate the selective adsorption properties of ionic polyimides and ionic polyimide/ionic liquid composites
- Generate and analyze molecular dynamics and structural analysis code
- Create three-dimensional representations of molecular simulation data utilizing design software and 3D printing

PROFICIENCIES

- | | |
|----------------------|---|
| • Platforms | Windows, Linux, OS X |
| • Programming | Fortran, Python, HTML |
| • Important Packages | Pytorch, Tensorflow, OpenMM, GROMACS, Cassandra |
| • 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 **2017** 33 (42), 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.jpcc.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

arXiv preprint arXiv:2208.10715 (2022).

University of Alabama Undergraduate Research Conference – Tuscaloosa, Alabama **March 2015**

- Poster, “Physical Representations of Molecular Simulation Data”

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”

HONORS AND AWARDS

Randall Outstanding Undergraduate Research Award

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

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

University of Alabama Presidential Merit Scholarship

- Full academic scholarship provided by the University of Alabama

Omega Chi Epsilon ($\Omega\chi\epsilon$)

- Chemical engineering honor society for the top percentile of chemical engineering students at the University of Alabama

Gamma Sigma Epsilon ($\Gamma\Sigma\epsilon$)

- Chemistry honor society for the top percentile of chemistry students at the University of Alabama

Phi Eta Sigma ($\Phi\eta\Sigma$)

- First year honor society that recognizes students' outstanding academic achievement in their first year of university