Natalie Malka Isenberg

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Education

University of Pittsburgh – B.S. Chemical Engineering (August 2016)

Carnegie Mellon University – Ph.D Chemical Engineering (August 2016 – December 2021)

Research Interests & Expertise

Mathematical modeling, mathematical optimization, mixed-integer linear programming (MILP), nonlinear programming, nonconvex optimization, materials design, catalysis, alternative energy technology, process systems engineering, robust optimization, machine learning, decision-making under uncertainty

Experience

Amalie Emmy Noether Postdoctoral Fellow, **Brookhaven National Laboratory, Computational Science Initiative**

(Fall 2021 – Present)

- **Uncertainty quantification** for biological pathway models for use in **generative molecular design**
- **Optimal experimental design** for improving model predictions of therapeutic ability
- **Bayesian calibration** and **discrepancy** modeling for optimal **quantum hardware design**

Graduate Student Researcher, **Gounaris Research Group, Carnegie Mellon University, Department of Chemical Engineering**

(Fall 2016 – Fall 2021)

- Formulating and solving **mathematical optimization models** to determine optimal **materials** for CO_2 adsorption
- **Developing Robust optimization** techniques for large-scale, non-convex **nonlinear** process models
- **Collaboration** with the National Energy Technology Laboratory (NETL) to create a robust optimization package in Python for the Institute for the Design of Advanced Energy Systems (IDAES) project

***Graduate Student Research Fellow*, U.S. DOE Office of Science Graduate Student Research Fellowship (SCGSR)**

(Spring 2020)

- Working with scientists while visiting at Sandia National Laboratories (SNL) Discrete Math and Optimization team to develop novel **robust optimization software**

Research Intern, **DAAD Research Internship in Science and Engineering (RISE)**

(Summer 2015)

- Awarded research internship in Germany to investigate effects of modified **ceramics** in energy storage processes

***Undergraduate Researcher*, Swanson School of Engineering, University of Pittsburgh, Dr. C. Wilmer**

(Fall 2015 – Fall 2016)

- Studied computational methods for chemical **gas sensors** using **metal organic frameworks**

***Research Intern*, Mascaro Center for Sustainable Innovation (MCSI), University of Pittsburgh, Dr. G. Veser**

(Summer 2013 – Summer 2014)

- Headed research project to test **dopants** in cerium dioxide **supports** for improved structural integrity and oxygen availability

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Journal Publications

1. S. Bhavsar, **N.M. Isenberg**, A. More, G. Veser, "Lanthana-doped ceria as active support for oxygen carriers in chemical looping combustion," *Applied Energy*, 2016. https://doi.org/10.1016/j.apenergy.2016.01.073
2. **N.M. Isenberg**, Z. Yan, M.G. Taylor, C.L. Hanselman, G. Mpourmpakis, C.E. Gounaris, "Identification of Optimally Stable Nanocluster Geometries via Mathematical Optimization and Density-Functional Theory," *Molecular Systems Design and Engineering,* 2019. https://doi.org/10.1039/C9ME00108E
3. **N.M. Isenberg,** P. Akula, J.C. Eslick, D. Bhattacharyya, D.C. Miller, C.E. Gounaris, "A Generalized Robust Cutting-Set Algorithm for Nonlinear Robust Optimization in Process Systems Engineering Applications," *AIChE Journal*, 2021. https://doi.org/10.1002/aic.17175
4. X. Yin, **N. M. Isenberg**, C. L. Hanselman, J. R. Dean, G. Mpourmpakis, C. E. Gounaris, "Designing stable bimetallic nanoclusters via an iterative two-step optimization approach," *Molecular Systems Design and Engineering,* 2021. https://doi.org/10.1039/d1me00027f
5. **N.M. Isenberg,** J.D. Siirola, C.E. Gounaris, "PyROS: A Pyomo Robust Optimization Solver for Robust Process Design," (In preparation), 2022.
6. **N.M. Isenberg,** S. Mertins, B.J. Yoon, K. Reyes, N. Urban, "Integrating HPC with Optimal Design of Experiments for Biological Pathway Models to Predict Inhibitor Efficacy," (In preparation), 2023.

Oral Presentations

- CORS/INFORMS International Conference (2022), *PyROS: A Cutting-set Based Robust Optimization Solver for Non-convex, Equality Constrained Problems in Python*, **N.M. Isenberg**, J. D. Siirola, C.E. Gounaris
- AIChE Annual Meeting (2021), *New Features and Comprehensive Benchmarking Study of the Pyomo Robust Optimization Solver (PyROS)*, **N.M. Isenberg**, J. D. Siirola, C.E. Gounaris
- INFORMS Annual Meeting (2021), *A Comprehensive Performance Study of the Pyomo Robust Optimization Solver (PyROS)*, **N.M. Isenberg**, J.D. Siirola, C.E. Gounaris
- AIChE Annual Meeting (2020), ***CAST Plenary Talk***, *Robust Optimization for Chemical Process Systems Engineering*, N.M. Isenberg, J.D. Siirola, **C.E. Gounaris**
- INFORMS Annual Meeting (2020), *PyROS: The Robust Optimization Solver Package for Pyomo*, **N.M. Isenberg**, J.D. Siirola, C.E. Gounaris
- INFORMS Annual Meeting (2019), *A Generalized Cutting Set Approach For Robust Process Design*, **N.M. Isenberg**, P. Akula, D. Bhattacharya, D.C. Miller, C.E. Gounaris
- AIChE Annual Meeting (2019), *Robust Optimization for Chemical Process Design and Applications to Carbon Capture Technology*, **N.M. Isenberg**, P. Akula, D. Bhattacharya, D.C. Miller, C.E. Gounaris
- AIChE Annual Meeting (2018), *Identification of Optimally Stable Nanocluster Geometries via Mathematical Optimization and Density-Functional Theory*, **N.M. Isenberg**, Z. Yan, M.G. Taylor, C.L. Hanselman, G. Mpourmpakis, C.E. Gounaris
- INFORMS Annual Meeting (2018), *Mathematical Optimization Based Approaches for the Design of Materials in Energy Applications* **C.E. Gounaris**, C.L. Hanselman, N.M. Isenberg

Invited Talks

- ICFA Workshop on Machine Learning (2022), *Tutorial on Uncertainty Quantification for Machine Learning*, **N.M. Isenberg**
- Rising Stars Workshop for Women in Computational and Data Science (2022), *Uncertainty Quantification and Optimal Experimental Design for Biological Pathway Models,* **N.M. Isenberg**
- AIChE Annual Meeting (2020), ***CAST Directors' Student Presentation Awards Finalist***, *Pyros: A Pyomo Robust Optimization Solver for Robust Process Design*, **N.M. Isenberg**, J. D. Siirola, C.E. Gounaris

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Relevant Coursework:

- Linear Programming
- Integer Programming
- Constraint Programming
- Introduction to Machine Learning
- Defects in Materials
- Special Topics: Process Systems Engineering
- Modern Convex Optimization

Volunteer and Leadership Experience

Outreach Coordinator, Carnegie Mellon University, Chemical Engineering Graduate Student Association(2017-2019)

- Coordinated and ran STEM related volunteer events for graduate students

Secretary, Pittsburgh-Cleveland Catalysis Society (PCCS), (2019-2021)

- Managed abstract submissions and communications for the PCCS Annual Research Meeting

Symposium Chair, Carnegie Mellon University, Chemical Engineering Graduate Student Association, (2018-2019)

- Organized annual student research symposium

Volunteer Judge, Pennsylvania Junior Academy of Science Region 7, (2017, 2018, 2019)

- Judged elementary and middle school student science fair presentations and determined special award recipients

Teaching Assistant (TA), Carnegie Mellon University, Department of Chemical Engineering

- Introduction to Chemical Engineering (Fall 2016)
- Optimization Modeling and Algorithms & Chemical Process Design (Spring 2017, Spring 2018, Spring 2019)

Volunteer Instructor, Propel EAST Middle School, (2015 - 2016)

- Taught a weekly introductory creative programming course to elementary and middle school students

Awards

Research Awards:

- Rising Stars for Women in Computational and Data Sciences Awardee (2022)
- Presidential Fellowship, Carnegie Mellon University College of Engineering Awardee (2020)
- DOE Office of Science Graduate Student Research Fellowship Awardee (2019)
- Foundations of Computer-Aided Process Design (FOCAPD) Poster Award Winner (2019)
- 2nd Place, EQT Optimization Poster Award, CAPD Annual Review Meeting (2019)
- Bayer/Covestro Award for outstanding undergraduate students in chemical engineering (2016)
- 1st place poster presentation at "Chemical Engineering Research Day" at the University of Pittsburgh (2015)
- 1st place for undergraduate research in the Mascaro Center for Sustainable Innovation Internship (2014)

Outreach Awards:

- Gelfand Student Service Award, Carnegie Mellon University (2019)

Teaching Awards:

- Mark Dennis Karl Outstanding Graduate Teaching Assistant Award, Carnegie Mellon University (2018)

Technical Skills

Programming Languages: C++, Python, Julia, Java, MATLAB

Optimization Software/Packages: IBM ILOG CPLEX, Gurobi, IPOPT/IPOPTH, BARON, GAMS, Pyomo