

Natalie Malka Isenberg

POSTDOCTORAL FELLOW OF APPLIED MATHEMATICS · BROOKHAVEN NATIONAL LABORATORY

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Education

Carnegie Mellon University

PHD CHEMICAL ENGINEERING

- Advisor: Dr. Chrysanthos E. Gounaris

Pittsburgh, PA

Aug. 2016 - Sept. 2021

University of Pittsburgh

BS CHEMICAL ENGINEERING

- Undergrad research advisor: Dr. Goetz Vesper

Pittsburgh, PA

2012 - 2016

Professional Experience

- 2021-2023 **Amalie Emmy Noether Postdoctoral Fellow**, Applied Mathematics, Brookhaven National Laboratory
- 2016-2021 **Graduate Research Assistant**, Department of Chemical Engineering, Carnegie Mellon University
- 2019 **DOE Office of Science Graduate Student Research (SCGSR) Research Fellow**, Sandia National Laboratories
- 2016-2020 **Graduate Teaching Assistant**, Department of Chemical Engineering, Carnegie Mellon University
- 2013-2016 **Undergraduate Research Assistant**, Department of Chemical Engineering, University of Pittsburgh

Publications

PUBLISHED

- 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.
- 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.
- 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.
- S. Bhavsar, **N.M. Isenberg**, A. More, G. Vesper, "Lanthana-doped Ceria as Active Support for Oxygen Carriers in Chemical Looping Combustion," *Applied Energy*, 2016.

IN PREP

- N.M. Isenberg**, J.D. Siirola, C.E. Gounaris, "PyROS: A Pyomo Robust Optimization Solver for Robust Process Design."
- N.M. Isenberg**, S. Mertins, B.J. Yoon, K. Reyes, N. Urban, "Integrating HPC with Optimal Design of Experiments for Biological Pathway Models."

Awards, Fellowships, & Grants

- 2021 **Amalie Emmy Noether Postdoctoral Fellowship**, Brookhaven National Laboratory
- 2021 **Rising Stars for Women in Computational and Data Sciences Awardee**, Sandia National Laboratory
- 2020 **Presidential Fellowship**, Department of Chemical Engineering, Carnegie Mellon University
- 2019 **Graduate Student Research Fellowship Awardee**, DOE Office of Science
- 2019 **Poster Award Winner**, Foundations of Computer-Aided Process Design (FOCAPD)

Presentations

INVITED TALKS

Fall 2022. *Uncertainty Quantification for Machine Learning*. Invited tutorial: ICFA Workshop on Machine Learning for Accelerator Beam Dynamics, Chicago, IL

Spring 2022. *Uncertainty Quantification for Computational Drug Discovery*. Invited talk: Rising Stars Workshop for Women in Computational and Data Science, Albuquerque, NM.

Fall 2020. *PyROS: A Pyomo Robust Optimization Solver for Robust Process Design*. Invited talk: CAST Directors' Student Presentation Awards Finalist, AIChE Annual Meeting, Virtual Meeting.

CONTRIBUTED PRESENTATIONS

N.M. Isenberg, J. D. Sirola, C.E. Gounaris. 2022. PyROS: A Cutting-set Based Robust Optimization Solver for Non-convex, Equality Constrained Problems in Python. Oral presentation: CORS/INFORMS International Conference, Vancouver, CA.

N.M. Isenberg, J. D. Sirola, C.E. Gounaris. 2021. New Features and Comprehensive Benchmarking Study of the Pyomo Robust Optimization Solver (PyROS). Oral presentation: AIChE Annual Meeting, Boston, MA.

N.M. Isenberg, J.D. Sirola, C.E. Gounaris. 2021. A Comprehensive Performance Study of the Pyomo Robust Optimization Solver. Oral presentation: INFORMS Annual Meeting, Anaheim, CA.

C.E. Gounaris, N.M. Isenberg. 2020. Robust Optimization for Chemical Process Systems Engineering. CAST Plenary Talk: AIChE Annual Meeting, Virtual Meeting.

N.M. Isenberg, J.D. Sirola, C.E. Gounaris. 2020. PyROS: The Robust Optimization Solver Package for Pyomo. Oral presentation: INFORMS Annual Meeting, Virtual Meeting.

N.M. Isenberg, P. Akula, D. Bhattacharya, D.C. Miller, C.E. Gounaris. 2019. A Generalized Cutting Set Approach For Robust Process Design. Oral presentation: INFORMS Annual Meeting, Seattle, WA.

N.M. Isenberg, P. Akula, D. Bhattacharya, D.C. Miller, C.E. Gounaris. 2019. Robust Optimization for Chemical Process Design and Applications to Carbon Capture Technology. Oral presentation: AIChE Annual Meeting, Orlando, FL.

N.M. Isenberg, P. Akula, D. Bhattacharya, J.C. Eslick, D.C. Miller, C.E. Gounaris. 2019. Robust Optimization for Nonlinear Chemical Process Models: Applications to Post-Combustion Carbon Capture. Poster: Foundations of Computer-Aided Process Design (FOCAPD), Denver, CO.

N.M. Isenberg, Z. Yan, M.G. Taylor, C.L. Hanselman, G. Mpourmpakis, C.E. Gounaris. 2018. Identification of Optimally Stable Nanocluster Geometries via Mathematical Optimization and Density-Functional Theory. Oral presentation: AIChE Annual Meeting, Pittsburgh, PA.

C.E. Gounaris, C.L. Hanselman, N.M. Isenberg. 2018. Mathematical Optimization Based Approaches for the Design of Materials in Energy Applications. Oral presentation: INFORMS Annual Meeting, Phoenix, AZ.

Research Experience

Brookhaven National Laboratory - Computational Science Initiative

ADVISOR: DR. NATHAN URBAN

Upton, NY

Oct. 2021 - Present

- Uncertainty quantification for biological pathway models for use in generative molecular design
- Optimal experimental design to improve model predictions of therapeutic ability for novel drug molecules
- Bayesian calibration and discrepancy modeling for optimal design of quantum hardware to minimize correlated errors

Carnegie Mellon University - Department of Chemical Engineering

ADVISOR: DR. CHRYSANTHOS E. GOUNARIS

Pittsburgh, PA

Aug. 2016 - Sept. 2021

- Dissertation: "Mixed-Integer Optimization for Nanomaterial Design and Optimization Under Uncertainty for Nonlinear Process Models"

Sandia National Laboratories - Discrete Math and Optimization

ADVISOR: DR. JOHN D. SIROLA

Albuquerque, NM

Spring 2020

- Project: Develop an open-source robust optimization solver in Pyomo for solving nonlinear uncertain optimization problems

University of Pittsburgh - Department of Chemical and Petroleum Engineering

Pittsburgh, PA

ADVISORS: DR. GOETZ VESER

2013-2016

- Project: Design improved oxygen carrier materials for chemical-looping combustion

Outreach & Professional Development

SERVICE AND OUTREACH

- 2017-2019 **Chemical Engineering Graduate Student Association**, Outreach Coordinator
- 2019-2021 **Pittsburgh-Cleveland Catalysis Society**, Secretary
- 2018-2019 **Chemical Engineering Graduate Student Association**, Symposium Chair
- 2017-2019 **Pennsylvania Junior Academy of Science**, Science Fair Judge
- 2016-2019 **Carnegie Mellon Department of Chemical Engineering**, Teaching Assistant
- 2015-2016 **Propel EAST Elementary and Middle School**, Volunteer Instructor

PEER REVIEW

Computers and Chemical Engineering
INFORMS Journal on Computing