Natalie Malka Isenberg

Postdoctoral Fellow of Applied Mathematics · Brookhaven National Laboratory

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Education

Carnegie Mellon University — *Pittsburgh, PA*
PhD Chemical Engineering — *Aug. 2016 - Sept. 2021*
- Advisor: Dr. Chrysanthos E. Gounaris

University of Pittsburgh — *Pittsburgh, PA*
BS Chemical Engineering — *2012 - 2016*
- Undergrad research advisor: Dr. Goetz Veser

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. Veser, "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 Accelarator 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. Siirola, 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. Siirola, 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. Siirola, 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. Siirola, 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 *Upton, NY*

Advisor: Dr. Nathan Urban *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 *Pittsburgh, PA*

Advisor: Dr. Chrysanthos E. Gounaris *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 *Albuquerque, NM*

Advisor: Dr. John D. Siirola *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