

## Ishan Bajaj

Department of Chemical Engineering, IIT Roorkee  
Tel. (637) · 851 · 2060, Email id. ishanbajaj567@gmail.com

### Research Interests

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- Algorithmic advancements in data-driven optimization and surrogate modeling
- Deterministic global optimization of nonconvex programming problems
- Hyper-parameter optimization for automatic machine learning
- Modeling and analysis of renewable energy systems
- Energy efficient and cost effective process design
- Modeling and optimization of strategies for decarbonizing chemical industry

### Education

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**Ph.D., Chemical Engineering, Texas A&M University** *Sep 2014 - Feb 2019*

Research topic: *Optimization Methods and Algorithms for Classes of Black-box and Grey-box Problems*

Advisor: *Professor M. M. Faruque Hasan*

**B.Tech., Chemical Engineering, Indian Institute of Technology, Bombay** *July 2009 - May 2013*

Research topic: *Design and Analysis of Signed Digraphs*

Advisor: *Professor Mani Bhushan*

### Professional Background

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**Indian Institute of Technology, Roorkee** *Apr 2022 - present*

Assistant Professor, Department of Chemical Engineering

**Princeton University** *Mar 2021- Mar 2022*

Postdoctoral Research Associate, Andlinger Center for Energy and the Environment

**University of Wisconsin-Madison** *Apr 2019- Feb 2021*

Postdoctoral Research Associate, Department of Chemical and Biological Engineering

### Awards and Honors

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- Distinguished Graduate Research Award, Department of Chemical Engineering, TAMU *2018*
  - One selected amongst more than 100 PhD students
- AIChE CAST Directors' Student Presentation Award Finalist *2018*
  - Eight PhD students selected from process systems engineering community worldwide
- Process Systems Engineering (PSE) 2018 Young Researcher Award *2018*
  - Travel support to attend PSE conference conducted every four years
  - Leading author of thirty papers were selected from four hundred and fifty papers
- First prize, Utilities Challenge, Texas A&M University *2018*
  - A total of four teams with diverse academic backgrounds participated
- Foundations of Computer Aided Process Operations (FOCAPO) Travel Award *2017*
- Research and Presentation Travel Award, OGAPS, Texas A&M University *2017*
- Best Session Paper, AIChE Annual Meeting, San Francisco, CA *2016*
- Fellow, Academy of Future Faculty, Texas A&M University *2015*
- Undergraduate Research Award, Indian Institute of Technology, Bombay *2012*

### Research Grants

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**Synergistic Thermo-Microbial-Electrochemical (T-MEC) Approach for Drop-In Fuel Production from Wet Waste**

- Co-authored a grant application along with research groups at Princeton University, University of Illinois at Urbana-Champaign, Pacific Northwest National Laboratory
- Grant application was accepted and awarded **\$2.5 million**

### Journal Publications (\* indicates equal contribution)

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*Published:*

1. **I. Bajaj** and M. M. F. Hasan. Global dynamic optimization using edge-concave underestimator. *Journal of Global Optimization*, 2020, 77(3), 487-512. (*IF=1.8*)
2. **I. Bajaj**, M. M. F. Hasan. Deterministic global derivative-free optimization of black-box problems with bounded Hessian. *Optimization Letters*, 2020, 14:1011-1026. (*IF=1.6*)
3. **I. Bajaj**, M. M. F. Hasan. UNIPOPT: Univariate projection-based optimization without derivatives. *Computers & Chemical Engineering*, 2019, 127, 71-87. (*IF=4.0*)
4. **I. Bajaj**, S. S. Iyer, M. M. F. Hasan. A trust region-based two phase algorithm for constrained black-box optimization with infeasible initial point. *Computers & Chemical Engineering*, 2018, 116, 306-321. (*IF=4.0*)
5. X. Peng\*, **I. Bajaj\***, M. Yao, T. W. Root, C. T. Maravelias. Solid-gas thermochemical energy storage strategies for concentrating solar power: optimization and system analysis. *Energy Conversion and Management*, DOI: 10.1016/j.enconman.2021.114636. (*IF=9.7*)
6. H. Chang\*, **I. Bajaj\***, A. H. Motagamwala, A. Somasundaram, G. W. Huber, C. T. Maravelias, and J. A. Dumesic. Sustainable production of 5-hydroxymethyl furfural from glucose for process integration with high fructose corn syrup infrastructure. *Green Chemistry*, 2021, 23, 3277-3288 (*Selected as Journal cover and as a HOT article of the year*) (*IF=9.4*)
7. L. Yu, K. Seabright, **I. Bajaj**, D. M. Alonso, C. Hsieh, M. Li, H. Chen, D. J. Keffer, S. Dai, Y. A. Gandomi, C. T. Maravelias, D. P. Harper. Performance and economic analysis of organosolv softwood and herbaceous lignins to activated carbons as electrode materials in supercapacitors. *Frontiers in Energy Research*, 2022 (accepted). (*IF=3.3*)
8. H. Chang, **I. Bajaj**, G. W. Huber, C. T. Maravelias, and J. A. Dumesic. Catalytic strategy for conversion of fructose to organic dyes, polymers, and liquid fuels. *Green Chemistry*, 2020, 22(16), 5285-5295. (*Selected as Journal cover*) (*IF=9.4*)
9. A. Arora, S. S. Iyer, **I. Bajaj**, M. M. F. Hasan. Optimal methanol production via sorption enhanced reaction process, *Industrial & Engineering Chemistry Research*, 2018, 57(42): 14143-14161. (*IF=3.6*)
10. A. Arora, **I. Bajaj**, S. S. Iyer, M. M. F. Hasan. Optimal synthesis of periodic sorption enhanced reaction processes with application to hydrogen production. *Computers & Chemical Engineering*, 2018, 115, 89-111. (*IF=4.0*)
11. P. Balasubramanian, **I. Bajaj**, M. M. F. Hasan. Simulation and optimization of reforming reactors for carbon dioxide using both rigorous and reduced models. *J. CO<sub>2</sub> Util.*, 2018, 23, 80-104. (*IF=6.0*)
12. S. S. Iyer, **I. Bajaj**, P. Balasubramanian, M. M. F. Hasan. Integrated carbon capture and conversion to produce syngas: novel process design, intensification and optimization. *Ind. & Eng. Chem. Res.*, 2017, 56(30): 8622-8648. (*IF=3.6*)

*In preparation:*

13. **I. Bajaj**, X. Peng, C. T. Maravelias. Material screening and property optimization for thermochemical energy storage in concentrated solar power.
14. L. Yu, K. Seabright, **I. Bajaj**, et al. Performance and economic analysis of KOH-activated supercapacitor carbon.

#### Peer-Reviewed Conference Publications

1. **I. Bajaj**, X. Peng, C. T. Maravelias. Material Screening for Thermochemical Energy Storage in Solar Power Systems. *Computer Aided Chemical Engineering*, 2021, 50, 179-184.
2. **I. Bajaj**, M. M. F. Hasan. A Projection-based, data-driven method for high-dimensional black-box optimization. *Computer Aided Chemical Engineering*, 2018, 44, 973-978.
3. **I. Bajaj**, M. M. F. Hasan. A Novel Derivative-free optimization method based on single dimension projection. *Proceedings of FOCAPO/CPC*, Tucson, AZ, 2017.
4. **I. Bajaj**, M. M. F. Hasan. Effective sampling, modeling and optimization of constrained black-box problems. *Computer Aided Chemical Engineering*, 2016, 38, 553-558.
5. S. Kolluri, **I. Bajaj**, M. Bhushan. Sensor network design for efficient fault diagnosis and signed digraph update. *Proceedings of DYCOPS*, Mumbai, India, 2013.

#### Patent

1. M. M. F. Hasan, S. S. Iyer, P. Balasubramanian, **I. Bajaj**, A. Arora. Integrated carbon capture and conversion for production of syngas. U.S. Patent No. 11229871, 2022.

## Book Chapter

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1. **I. Bajaj**, A. Arora and M. M. F. Hasan. Advances in Black-box optimization. In P. Pardalos, M. Vrahatis and V. Rasskazova (Eds.), *Black Box Optimization, Machine Learning and No-Free Lunch Theorems*, 2021, 35-65.

## Invited Talks

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1. Indian Institute of Technology, Roorkee, UK, India, 2021. “Data-driven modeling and optimization for process intensification, material screening, and renewable chemicals production”.
2. Air Products, Allentown, PA, USA, 2021. “Modeling, Analysis and Optimization of Solar Power Systems, Biomass Conversion Pathways and Process Intensification”.
3. ExxonMobil Research and Engineering, Annandale, NJ, USA, 2018. “Optimization methods and algorithms for constrained black-box problems”.
4. The Dow Chemical Company, Lake Jackson, TX, USA, 2018. “Optimization methods for data-driven process systems”.
5. Workshop on Data-driven model reduction, scientific frontiers, and applications, Texas A&M University, College Station, TX, 2018. “Computational experience with different reduced models for derivative-free optimization”.

## Research Presentations

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1. **I. Bajaj**, X. Peng, C. T. Maravelias. An optimization-based framework for material selection and system design for integrating thermochemical energy storage in solar power systems. In *AIChE Annual Meeting*, Boston, MA, 2021.
2. **I. Bajaj**, X. Peng, C. T. Maravelias. System Design and Material Selection for Thermochemical Energy Storage in Solar Power Systems. In *Virtual 3rd Solar Energy Systems Conference*, 2021.
3. **I. Bajaj**, X. Peng, C. T. Maravelias. Reaction screening for Thermochemical Energy Storage. In *Virtual AIChE Annual Meeting*, 2020.
4. H. Chang, **I. Bajaj**, G. W. Huber, C. T. Maravelias, J. A. Dumesic. Catalytic Reaction Pathways and Process Synthesis for Biomass Conversion to High-value Chemicals for Organic Dye and Polymer Applications. In *Virtual AIChE Annual Meeting*, 2020.
5. H. Chang, **I. Bajaj**, G. W. Huber, C. T. Maravelias, J. A. Dumesic. Synthesis of a platform chemical for polymers and fuels industries via biomass-derived 5-hydroxymethyl furfural. In *Thermal & Catalytic Sciences Symposium*, Kennewick, WA, 2020.
6. **I. Bajaj**, M. M. F. Hasan. UNIPOPT: Univariate Projection-Based Optimization without Derivatives. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018. (*Received AIChE CAST Directors’ Student Presentation Finalist Award*)
7. **I. Bajaj**, S. S. Iyer, A. Arora, M. M. F. Hasan. Data-driven Optimization for Process Intensification Governed by High-Fidelity Models. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
8. **I. Bajaj**, M. M. F. Hasan. Global Optimization of a Class of Black-box Problems with Bounded Hessian. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
9. **I. Bajaj**, M. M. F. Hasan. New Underestimator and Branching Scheme for the Global Optimization of General Nonconvex Problems. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
10. S. S. Iyer, **I. Bajaj**, M. M. F. Hasan. Inverse Design of Nanoporous Adsorbents for Gas Separation Applications. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
11. A. Arora, **I. Bajaj**, S. S. Iyer, M. M. F. Hasan. Design and Optimization of Multifunctional Processes for Utilizing Unconventional and Distributed Feedstocks. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
12. A. Arora, S. S. Iyer, **I. Bajaj**, M. M. F. Hasan. Design and Intensification of Sorption-Enhanced Reaction Processes for Methanol Production. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
13. S. S. Iyer, **I. Bajaj**, M. M. F. Hasan. Process Optimization-Centric Design and Screening of Nanoporous Adsorbents for Gas Separations. In *AIChE Annual Meeting*, Pittsburgh, PA, 2018.
14. **I. Bajaj**, M. M. F. Hasan. A Projection-based, data-driven method for high-dimensional black-box optimization. In *Process Systems Engineering, PSE2018*, San Diego, CA, 2018. (*Received a PSE Young Researcher Award*)
15. P. Balasubramanian, **I. Bajaj**, M. M. F. Hasan. A process systems engineering perspective on CO<sub>2</sub>

- capture and utilization to produce chemicals. In *ICChE*, Dhaka, Bangladesh, 2017.
16. **I. Bajaj**, M. M. F. Hasan. A predictor-corrector algorithm for projection-based derivative-free optimization. In *AIChE Annual Meeting*, Minneapolis, MN, 2017.
  17. **I. Bajaj**, M. M. F. Hasan. Data-driven approximation of feasible region, constrained design of experiments, and optimization. In *AIChE Annual Meeting*, Minneapolis, MN, 2017.
  18. S. S. Iyer, **I. Bajaj**, M. M. F. Hasan. Design and intensification of integrated carbon capture and conversion to chemicals. In *AIChE Annual Meeting*, Minneapolis, MN, 2017.
  19. P. Balasubramanian, **I. Bajaj**, M. M. F. Hasan. CO<sub>2</sub> capture and conversion to chemicals via syngas: reactor modeling, process synthesis and optimization. In *AIChE Annual Meeting*, Minneapolis, MN, 2017.
  20. **I. Bajaj**, S. S. Iyer, P. Balasubramanian, M. M. F. Hasan. A Two-phase Derivative-free Optimization Algorithm for a Process Governed by Non-linear Algebraic Partial Differential Equations. In *INFORMS Annual Meeting*, Houston, TX, 2017.
  21. **I. Bajaj**, M. M. F. Hasan. Feasibility mapping and optimization using big data. in *AIChE Spring Meeting*, San Antonio, TX, 2017.
  22. **I. Bajaj**, M. M. F. Hasan. A Novel Derivative-free optimization method based on single dimension projection. In FOCAP/CPC, Tucson, AZ, 2017. (*Received FOCAP/CPC Travel Award*)
  23. P. Balasubramanian, **I. Bajaj**, M. M. F. Hasan. CO<sub>2</sub> capture and conversion to chemicals via syngas: rigorous modeling, intensification and superstructure-based process synthesis. In *AIChE Annual Meeting*, San Francisco, CA, 2016.
  24. **I. Bajaj**, M. M. F. Hasan. Optimization of constrained and multidimensional black-box problems using convex hull approximation and single dimension surrogate model. In *AIChE Annual Meeting*, San Francisco, CA, 2016.
  25. S. S. Iyer, P. Balasubramanian, **I. Bajaj**, M. M. F. Hasan. Design and optimization of integrated carbon capture and conversion with natural gas to produce syngas. In *AIChE Annual Meeting*, San Francisco, CA, 2016.
  26. Y. Shastri, **I. Bajaj**, S. Mittal, L. Rodriguez, and Y. Ouyang. Optimization of wheat supply chain for post-harvest loss minimization in India. In *49<sup>th</sup> Annual Convention of Indian Society of Agricultural Engineers and Symposium on Engineering Solutions for Sustainable Agriculture and Food Processing*, Ludhiana, India, 2015.

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## Leadership Experience and Professional Service

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| <b>Team Leader, Utilities Challenge, TAMU</b>   | <i>Feb 2018 - Apr 2018</i> |
| <ul style="list-style-type: none"> <li>• Led a 6 member team to research the utilities consumption of a dorm and improved its sustainability</li> </ul>   |                            |
| <b>Vice President, Texas A&amp;M Energy Research Society</b>  | <i>Oct 2016 - Oct 2017</i> |
| <ul style="list-style-type: none"> <li>• Led sponsorship outreach efforts resulting in 67% increase in sponsors and raised more than \$20,000</li> </ul>  |                            |
| <b>Organizing Committee, Texas A&amp;M Conference on Energy</b>   | <i>Oct 2016 - Oct 2017</i> |
| <ul style="list-style-type: none"> <li>• Organized a three-day Texas A&amp;M Conference on Energy with over 600 attendees and managed the expenses of the conference</li> </ul>   |                            |
| <b>Research mentoring, PU, UW-Madison, TAMU</b>   | <i>2016 - present</i>      |
| <ul style="list-style-type: none"> <li>• Mentored junior graduate students, undergraduate researchers, and research interns (Priyadarshini Balasubramanian, Logan Duran, Mihir Annaldasula, Ashis Patel, Shirene Singh, Arun Somasundaram)</li> </ul> |                            |

## Journal Manuscript Review

- Joule, Energy and Environment Science, Nature Sustainability, Mathematics, Journal of Global Optimization, Industrial and Engineering Chemistry Research, Energy Technology, Sustainability, Computers and Operations Research, Computers and Chemical Engineering, Applied Energy

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## Teaching

### Teaching assistant, Texas A&M University

- Chemical Engineering Fluid Operations and Chemical Engineering Mass Transfer Operations
- Graded quizzes and conducted help sessions

**Teaching volunteer, Princeton University**

- Prepared a project assignment for a senior undergraduate/graduate-level course (Optimization for the design and analysis of energy systems) based on my research

**Other Professional Activities**

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- Member, American Institute of Chemical Engineers (AIChE) *2016 - Present*
- Member, Institute for Operations Research and the Management Sciences (INFORMS) *2017 - Present*
- Session Chair, Texas A&M Conference on Energy *2016 - 2017*
- Session Judge, ChEGSA Research Symposium, Texas A&M University *2018*
- Student Leader, Finance and External Outreach Committee, Texas A&M Energy Research Society *2016*
- Session Judge, Student Research Week, Texas A&M University *2016*
- Organizer, 10<sup>th</sup> International Symposium on Dynamics and Control of Process System, Mumbai, India *2013*