Ananth Govind Rajan

Assistant Professor
Department of Chemical Engineering
Indian Institute of Science
CV Raman Avenue, Bengaluru
Karnataka 560012, India

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Professional Experience

08/2020 – present **Assistant Professor, Department of Chemical Engineering, Indian Institute of Science**

Research Areas: Computational nanotechnology for applications at the water-energy nexus, molecular simulations, density functional theory, machine learning, water/ion transport, electrocatalysis, energy storage, sustainable hydrogen production, electrochemical CO_2 reduction, synthesis of 2D materials

03/2019 – 08/2020 **Postdoctoral Research Associate, Department of Mechanical and Aerospace Engineering, Princeton University**

Advisor: Prof. Emily A. Carter

Research Areas: Computational catalysis, transition-metal-oxide electrocatalysts for water splitting, quantum-mechanical simulations of materials

Education

2019 **Ph.D. in Chemical Engineering, Massachusetts Institute of Technology**

Advisors: Prof. Daniel Blankschtein and Prof. Michael S. Strano

Thesis Title: "Atomistic Modeling and Simulations of 2D Materials: Chemical Vapor Deposition, Nanoporous Defects, Force-Field Development, Wetting, and Friction"

2015 **M.S. in Chemical Engineering Practice, Massachusetts Institute of Technology**
GPA: 4.8/5.0

2013 **B.Tech. in Chemical Engineering, Indian Institute of Technology Delhi**
CGPA: 9.82/10.0 (1st position in the department, awarded the Institute Silver Medal; 2nd in the institute)

Selected Honors & Awards

2023 **Infosys Young Investigator**, Division of Mechanical Sciences, Indian Institute of Science
2023 Invited to the **2023 Class of Influential Researchers**, Industrial and Engineering Chemistry Research
2023 **Guest Editor** for a special issue on "Materials Design" in the journal **ACS Engineering Au**
2023 Special issue article featuring **Early-Career & Emerging Researchers in Physical Chemistry** by The Journal of Physical Chemistry
2022 **International Travel Support** from the Science and Engineering Research Board (SERB), Government of India
2021 **Semi-Finalist** for MIT Technology Review's **Innovators Under 35 Award**
2019 Selected for the AIChE Education Division's **Future Faculty Mentoring Program**
2018 **1st Prize, Carbon Nanomaterials Graduate Student Award** at the Annual 2018 AIChE Meeting
2018 **MIT Graduate Student Council's Travel Award** to attend the 2018 AIChE Meeting
2016 **Dow Travel Award for Professional Development**, MIT to attend the AIChE 2016 Meeting
2015 **Rosemary J. Wojtowicz Award**, David H. Koch School of Chemical Engineering Practice, MIT

for recognition of personal generosity, integrity, and commitment

2013 **Landau ChE Practice School Fellowship**, Department of Chemical Engineering, MIT awarded to a first year PhD student

2013 **Institute Silver Medal**, IIT Delhi for securing the highest GPA among 65 graduating chemical engineering students

2013 **Amit Garg Memorial Ethical Leadership Award**, IIT Delhi for recognition of student leadership

2011 **Indian Academy of Sciences Summer Fellowship** for conducting research at the Institute of Chemical Technology, Mumbai

2009 CBSE **All India Engineering Entrance Examination Scholarship** (rank 97)

Publications (§ indicates equal contribution; * indicates corresponding author)

1. John, A., Verma, A. M., Shaneeth, M., **Govind Rajan, A.*** Discovering a Single-Atom Catalyst for CO_2 Electroreduction to C_1 Hydrocarbons: Thermodynamics and Kinetics on Aluminum-Doped Copper. *ChemCatChem*, In Press, DOI: 10.1002/cctc.202300188.

2. Seal, A., Tiwari, U., Gupta, A., **Govind Rajan, A.*** Incorporating Ion-Specific van der Waals and Soft Repulsive Interactions in the Poisson-Boltzmann Theory of Electrical Double Layers. *Phys. Chem. Chem. Phys.*, Under Revision.

3. Bhowmik, S., Warner, J. H., **Govind Rajan, A.*** Role of Chemical Etching in the Nucleation of Nanopores in 2D MoS_2: Insights from First-Principles Calculations. *J. Phys. Chem. C* **2023**, 127 (14), pp 6873–6883. (*Published in the special issue on "Early-Career and Emerging Researchers in Physical Chemistry Volume 2"*.)

4. Thomas, S., Silmore, K., Sharma, P., **Govind Rajan, A.*** Enumerating Stable Nanopores in Graphene and their Geometrical Properties Using the Combinatorics of Hexagonal Lattices. *J. Chem. Inf. Model.* **2023**, 63 (3), pp 870–881.

5. Kozawa, D.; Li, S. X.; Ichihara, T.; Rajan, A. G.; Gong, X.; He, G.; Koman, V. B.; Zeng, Y.; Kuehne, M.; Silmore, K. S.; Parviz, D.; Liu, P.; Liu, A. T.; Faucher, S.; Yuan, Z.; Warner, J.; Blankschtein, D.; Strano, M. S. Discretized Hexagonal Boron Nitride Quantum Emitters and Their Chemical Interconversion. *Nanotechnology* **2023**, *34*, 115702.

6. Verma, A. K., Verma, A. M., **Govind Rajan, A.*** Theoretical Understanding of Electrochemical Phenomena in 2D Electrode Materials. *Curr. Opin. Electrochem.* **2022**, 36, pp 101116.

7. Verma, A. K., **Govind Rajan, A.*** Surface Roughness Explains the Observed Water Contact Angle and Slip Length on 2D Hexagonal Boron Nitride. *Langmuir* **2022**, 38 (30), pp 9210–9220. (*This article was amongst the most-read ones in Langmuir a month after its publication*.)

8. Sheshanarayana, R., **Govind Rajan, A.*** Tailoring Nanoporous Graphene Via Machine Learning: Predicting Probabilities and Formation Times of Arbitrary Nanopore Shapes. *J. Chem. Phys*. **2022**, 156, 204703. (*This article is a part of the "Emerging Investigators Special Collection"* and was selected as an *"Editor's Pick".*)

9. Sharma, B. B., **Govind Rajan, A.*** How Grain Boundaries and Interfacial Electrostatic Interactions Modulate Water Desalination Via Nanoporous Hexagonal Boron Nitride. *J. Phys. Chem. B* **2022**, 126 (6), pp 1284–1300.

10. Bhowmik, S., **Govind Rajan, A.*** Chemical Vapor Deposition of 2D Materials: A Review of Modeling, Simulation, and Machine Learning Studies. *iScience* **2022**, 25 (3), 103832. (*This review was an invited article as part of the special issue titled "2D materials synthesis and processing strategies".*)

11. Seal, A., **Govind Rajan, A.*** Modulating Water Slip Using Atomic-Scale Defects: Friction on Realistic Hexagonal Boron Nitride Surfaces. *Nano Lett.* **2021**, 21 (19), pp 8008–8016.

12. **Govind Rajan, A.*,** Martirez, J. M. P., Carter, E. A.* Coupled Effects of Temperature, Pressure, and pH on Water Oxidation Thermodynamics and Kinetics. *ACS Catal.* **2021**, 11 (18), pp 11305–11319.

13. Yuan, Z., **Govind Rajan, A.**, He, G., Misra, R. P., Strano, M. S., Blankschtein, D.* Predicting Gas Separation through Graphene Nanopore Ensembles with Realistic Pore Size Distributions. *ACS Nano*, **2021**, 15 (1), pp 1727–1740.

14. Gupta, A., **Govind Rajan, A.**, Carter, E. A., Stone, H. A.* Thermodynamics of Electrical Double Layers with Electrostatic Correlations. *J. Phys. Chem. C*, **2020**, 124 (49), pp 26830–26842.

15. Gupta, A., **Govind Rajan, A.**, Carter, E. A., Stone, H. A.* Ionic Layering and Overcharging in Electrical Double Layers in a Poisson-Boltzmann Model. *Phys. Rev. Lett.*, **2020**, 125 (18), pp 188004.

16. **Govind Rajan, A.**, Carter, E. A.* Microkinetic Model for pH- and Potential-Dependent Oxygen Evolution During Water Splitting on Fe-Doped β-NiOOH. *Energy Environ. Sci.*, **2020**, 13, pp 4962–4976. (*This article is part of the themed collection:* 2020 Energy and Environmental Science HOT Articles.)

17. **Govind Rajan, A.**, Carter, E. A.* Discovering Competing Electrocatalytic Mechanisms and their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways. *J. Phys. Chem. C*, **2020**, 124 (25), pp 24883–24898.

18. **Govind Rajan, A.**, Martirez, J. M. P., Carter, E. A.* Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)electrochemical Water Splitting? *ACS Catal.*, **2020**, 10 (19), pp 11177–11234.

19. **Govind Rajan, A.**, Martirez, J. M. P., Carter, E. A.* Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH: Different Chemistries Leading to Similar Overpotentials. *J. Am. Chem. Soc.*, **2020**, 142 (7), pp 3600–3612.

20. Dong, J., Lee, M. A., **Govind Rajan, A.**, Rahaman, I., Sun, J. H., Park, M., Salem, D. P., Strano, M. S.* A Synthetic Mimic of Phosphodiesterase Type 5 Based on Corona Phase Molecular Recognition Using Single Walled Carbon Nanotubes. *Proc. Natl. Acad. Sci. USA*, **2020**, 117 (43), pp 26616–26625.

21. Yuan, Z., Misra, R. P., **Govind Rajan, A.**, Strano, M. S., Blankschtein, D.* Analytical Prediction of Gas Permeation through Graphene Nanopores of Varying Sizes: Understanding Transitions across Multiple Transport Regimes. *ACS Nano*, **2019**, 13 (10), pp 11809–11824.

22. Wang., S., Zhang, Z., Zhang, H., **Govind Rajan, A.**, Xu, N., Yang, Y., Zeng, Y., Liu, P., Zhang, X., Mao, Q., He, Y., Zhao, J., Li, B.-G., Strano, M. S., Wang, W.-J.* Reversible Polycondensation-Termination Growth of Covalent-Organic-Framework Spheres, Fibers, and Films Consisting of Interweaved Nanoflakes. *Matter*, **2019**, 1 (6), pp 1592–1605.

23. Faucher, S., Aluru, N., Bazant, M. Z., Blankschtein, D., Brozena, A. H., Cumings, J., de Souza, J. P., Elimelech, M., Epsztein, R., Fourkas, J. T., **Govind Rajan, A.**, Kulik, H. J., Levy, A., Majumdar, A., Martin, C., McEldrew, M., Misra, R. P., Noy, A., Pham, T. A., Reed, M., Schwegler, E., Siwy, Z., Wang, Y., Strano, M. S.* Critical Knowledge Gaps in Mass Transport Through Single-Digit Nanopores: A Review and Perspective. *J. Phys. Chem. C*, **2019**, 123 (35), pp 21309–21326.

24. Arash, A., Ahmed, T., **Govind Rajan, A.**, Walia, S., Mazumder, A., Ramanathan, R., Sriram, S., Bhaskaran, M., Strano, M. S., Balendhran, S.* Large-Area Synthesis of Two-Dimensional MoO_{3-x} for Enhanced Optoelectronic Applications. *2D Mater.*, **2019**, 6, pp 035031.

25. Li, R., Antunes, E. F., Cohen, E., Kudo, A., Acauan, L., Yang, W.-C. D., Wang, C., Cui, K., Liotta, A., **Govind Rajan, A.,** Gardener, J., Bell, D. C., Strano, M. S., Liddle, A. Sharma, R., Wardle, B.* Low-Temperature Growth of Carbon Nanotubes Catalyzed by Sodium-based Household Ingredients. *Angew. Chemie. Int. Ed.*, **2019**, 58, pp 1–7. (*this work was featured on the MIT Homepage, http://web.mit.edu/archive/spotlight/new-recipe-nanotubes/, on MIT News,*

http://news.mit.edu/2019/ingredients-grow-carbon-nanotubes-0529, and on other news outlets, such as Phys.org)

26. **Govind Rajan, A.**, Strano, M. S., Blankschtein, D.* Liquids with Lower Wettability Can Exhibit Higher Friction on Hexagonal Boron Nitride: The Intriguing Role of Solid-Liquid Electrostatic Interactions. *Nano Lett.*, **2019**, 19 (3), pp 1539–1551.

27. Cardellini, A., Alberghini, M., **Govind Rajan, A.**, Misra, R. P., Blankschtein, D.*, Asinari, P*. Multi-Scale Approach for Modeling Stability, Aggregation, and Network Formation of Nanoparticles Suspended in Aqueous Solutions. *Nanoscale*, **2019**, 11, pp 3979–3992.

28. Drahushuk, L. W.[§], **Govind Rajan, A.[§]**, Strano, M. S.* Fundamental Scaling Laws for the Direct-Write Chemical Vapor Deposition of Nanoscale Features: Modeling Mass Transport Around a Translating Nanonozzle. *Nanoscale*, **2019**, 11, pp 2925–2937.

29. **Govind Rajan, A.**, Silmore, K., Swett, J., Blankschtein, D., Strano, M. S.* Addressing the Isomer Cataloging Problem for Nanopores in Two-Dimensional Materials. *Nat. Mater.*, **2019**, 18, pp 129–135. (*this work was featured on the MIT Homepage, http://web.mit.edu/spotlight/cataloging-graphene-defects/, on MIT News, http://news.mit.edu/2019/catalog-atom-vacancy-2-d-materials-0114, and on other news outlets, such as Phys.org; this work appeared in an appendix to the National Nanotechnology Initiative Supplement to the United States President's 2020 Budget.*)

30. **Govind Rajan, A.**, Strano, M. S., Blankschtein, D.* Ab Initio Molecular Dynamics and Lattice Dynamics Based Force Field to Model Hexagonal Boron Nitride in Mechanical and Interfacial Applications. *J. Chem. Phys. Lett.*, **2018**, 9, pp 1584–1591.

31. Yuan, Z., **Govind Rajan, A.**, Misra, R. P., Drahushuk, L.W., Agrawal, K. V., Strano, M.S., Blankschtein, D.* Mechanism and Prediction of Gas Permeation through Sub-Nanometer Graphene Pores: Comparison of Theory and Simulation, *ACS Nano*, **2017**, 11 (8), pp 7974-7987.

32. Kaplan, A., Yuan, Z., Benck, J.D., **Govind Rajan, A.**, Chu, X.S., Wang, Q.H.*, Strano, M.S.* Current and Future Directions in Electron Transfer Chemistry of Graphene. *Chem. Soc. Rev.*, **2017**, 46, pp 4530-4571.

33. Agrawal, K. V., Benck, J. D., Yuan, Z., Misra, R. P., **Govind Rajan, A.**, Eatmon, Y., Kale, S., Chu, X. S., Li, D. O., Gong, C., Warner, J., Wang, Q. H., Blankschtein, D., Strano, M. S.* Fabrication, Pressure Testing, and Nanopore Formation of Single-Layer Graphene Membranes. *J. Phys. Chem. C*, **2017**, 121 (26), pp 14312-14321.

34. Lin, S.[§], Shih, C.-J.[§], Sresht, V.[§], **Govind Rajan, A.[§]**, Strano, M. S., Blankschtein, D.* Understanding the Colloidal Dispersion Stability of 1D and 2D Materials: Perspectives from Molecular Simulations and Theoretical Modeling. *Adv. Colloid Interface Sci.* **2017**, 244, pp. 36-53.

35. Sresht, V.[§], **Govind Rajan, A.[§]**, Bordes, E., Strano, M. S., Padua, A. A. H.*, Blankschtein, D.* Quantitative Modeling of MoS_2 – Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics. *J. Phys. Chem. C*, **2017**, 121 (16) pp 9022-9031. *(This work was featured on the cover page of The Journal of Physical Chemistry C, http://pubs.acs.org/toc/jpccck/121/16.)*

36. **Govind Rajan, A.**, Sresht, V., Padua, A. A. H., Strano, M. S., Blankschtein, D.* Dominance of Dispersion Interactions and Entropy Over Electrostatics in Determining the Wettability and Friction of Two-Dimensional MoS_2 Surfaces. *ACS Nano*, **2016**, 10 (10), pp 9145-9155.

37. Ulissi, Z. W., **Govind Rajan, A.**, Strano, M. S.* Persistently Auxetic Materials: Engineering the Poisson Ratio of 2D Self-Avoiding Membranes under Conditions of Non-Zero Anisotropic Strain. *ACS Nano*, **2016**, 10 (8), pp 7542-7549.

38. **Govind Rajan, A.**, Warner, J. H., Blankschtein, D., Strano, M. S.* Generalized Mechanistic Model for the Chemical Vapor Deposition of 2D Transition Metal Dichalcogenide Monolayers. *ACS Nano*, **2016**, 10 (4), pp 4330-4344.

39. Son, Y., Wang, Q. H., Paulson, J. A., Shih, C.-J., **Rajan, A. G.**, Tvrdy, K., Kim, S., Alfeeli, B., Braatz, R. D., Strano, M. S.* Layer Number Dependence of MoS_2 Photoconductivity Using Photocurrent Spectral Atomic Force Microscopic Imaging. *ACS Nano*, **2015**, 9 (3), pp 2843-2855.

Patents

1. Govind Rajan, A., Martirez, J. M. P., Carter, E. A. "A Method of Generating Oxygen by Electrochemical Water Splitting at Optimized Conditions of pH, Temperature, and Pressure" (complete Indian patent 430439 granted on 28-04-2023; PCT/IB2022/057592 published on 16-02-2023)

Service to the Scientific Community

- **Reviewer** for *Nature Catalysis, ACS Catalysis, ACS Nano*, *ACS Energy Letters*, *Nature Communications*, *npj 2D Materials and Applications*, *Journal of Chemical Physics*, *The Journal of Physical Chemistry*, *The Journal of Physical Chemistry Letters*, *ChemCatChem*, *ChemPhysChem*, *Journal of Chemical Information and Modeling*, *ACS Applied Materials & Interfaces*, *Advanced Energy Materials, Phys. Chem. Chem. Phys., Physical Review B, Journal of Applied Physics*, *Crystal Growth and Design*, *Computational Materials Science*

- **Session chair** for:
  - CO_2 Upgrading: From Fundamental to Applied CO2 Electrocatalysis, AIChE 2022 Annual Meeting
  - Electrocatalysis and Photoelectrocatalysis (Virtual), AIChE 2021 Annual Meeting
  - Soft Matter Young Investigators e-Meet 2020

- **Judge** for:
  - Poster presentation, Catalysis and Reaction Engineering Division, AIChE 2022 Annual Meeting
  - Poster presentation, ACS Spring 2022 and Fall 2021 India Satellite Meetings

- **Guest editor** for:
  - Special issue on "Materials Design" by ACS Engineering Au (with Prof. Paul Dauenhauer, University of Minnesota, Twin Cities and Dr. Steven Arturo, Dow Chemical Company)

- **Organizer** for:
  - *ChemE @ IISc 2022 Symposium*, celebrating the 75th year of the Department of Chemical Engineering at IISc, Bengaluru, with 15 invited speakers from across the country, including from IIT Delhi, IIT Madras, IIT Bombay, IIT Kanpur, IIT Guwahati, JNCASR, IIT Gandhinagar, NCBS, Shell, Reliance, Samsung R&D, and MolBio Diagnostics. (December 2022)

  - *New Approaches and Machine learning methods for Ab initio simulations (NAMMA) 2023*, in collaboration with Psi-k, with 8 international speakers and 20 Indian speakers working in the areas of (i) New Directions in First-Principles Methods and Techniques, (ii) Computational Design of Energy Materials, (iii) AI/ML for Ab Initio Simulations and Materials Discovery, and (iv) Quantum Materials and Algorithms. (July 2023)

Students/Postdoctoral Scholars/Project Associates Trained

- **Current:**
  1. Dr. Bharat Bhushan Sharma, Postdoctoral Research Associate
  2. Dr. Anand Mohan Verma, Postdoctoral Research Associate
  3. Dr. Sagar Ghorai, Postdoctoral Research Associate
  4. Ankit Kumar Verma, Ph.D. Student
  5. Dhondi Pradeep, Ph.D. Student
  6. Shivam Chaturvedi, Ph.D. Student

7. Pasyanthi Jampala, Ph.D. Student
8. Shiv Kumar, M.Tech. (Research) Student
9. Madhavan Nampoothiri, M.Tech. (Research) Student
10. Srinibas Nandi, M.Tech. Student
11. Piyush Sharma, M.Tech. Student
12. Anusha Tripathi, M.Tech. Student
13. Dhruv Lal, Project Associate
14. Sneha Thomas, M.S. Student (IISER Bhopal)
15. Aniruddha Seal, M.S. Student (NISER Bhubhaneswar)
16. Anshika Kushwaha, Undergraduate Student (Bundelkhand Institute of Engineering and Technology)

- **Alumni:**

  - **MTech (Res) Students**

Name	Position	Onward Position
Ashutosh Kumar Verma	M.Tech. (Research) Student (2021-22)	PhD Student, Oklahoma State University

  - **MTech Students**

Name	Position	Onward Position
Anwin John	M.Tech. Student (2021-22)	PhD Student, Purdue University
Sayan Bhowmik	M.Tech.Student (2021-22)	PhD Student, Georgia Institute of Technology

  - **Project Associates**

Name	Position	Onward Position
Tanmay Konnur	Project Associate (2021-22)	Masters Student, University of California, Los Angeles
Shubhani Paliwal	Undergraduate Student (2020-21); Project Associate (2021)	Masters Student, Imperial College London, UK

  - **Undergraduate Students**

Name	Position	Onward Position
Rahul Sheshanarayana	Undergraduate Student (2020-22)	Masters Student, Cornell University
Vineet Chandra Gokhale	Undergraduate Student (2020-22)	Analyst, Deloitte USI
Saswat Kumar Nayak	Undergraduate Student (2021)	Data Analyst, Innovaccer Analytics PhD Student, University of Wisconsin-Madison
Utkarsh Tiwari	Undergraduate Student (2020-21)	Process Safety Engineer, Exxon Mobil

  - **Summer Interns**

Name	Position	Onward Position
Mahika Nair	Summer Intern (2022)	Undergraduate Student, Krea University
Rohith Pulluri	Summer Intern (2022)	Undergraduate Student, Osmania University

Memberships of Professional Societies

- American Institute of Chemical Engineers (Senior Member)
- Indian Institute of Chemical Engineers (Lifetime Member)
- Royal Society of Chemistry (Member), MRSC
- American Chemical Society (Member)
- Materials Research Society (Member)
- Institution of Engineers, India (Associate Member)

Invited Talks

May 2023 "Single-Atom Alloys for CO_2 Reduction to C_1 Hydrocarbons on Cu(111): Thermodynamics and Kinetics on Al-Doped Copper," *Southeast Asian Catalysis Conference*, National University of Singapore, Singapore

May 2023 "Nanopores in 2D Materials: Understanding their Formation and Effects on Water/Ion Transport," *School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University (NTU)*, Singapore

Feb. 2023 "Probing Realistic Water-2D Material Interfaces Via Combined Quantum & Classical Simulations," *Lennard-Jones Centre, University of Cambridge*, Cambridge, United Kingdom (online)

Feb. 2023 "Nanopores in 2D Materials: Understanding their Formation and Effects on Water/Ion Transport," *Scientific Image Analysis and Simulations Team, Shell Technology Center Bengaluru*, India

Jan. 2023 "Nanopores in 2D Materials: Understanding their Formation and Effects on Water/Ion Transport," *Department of Materials Science and Engineering, Indian Institute of Technology Delhi*, New Delhi, India

Dec. 2022 "Single-Atom Alloys for CO_2 Reduction to C_1 Hydrocarbons on Cu(111): Thermodynamics and Kinetics on Al-Doped Copper," *Designing Catalysts on Computers (DCC) Meeting*, Indian Association for the Cultivation of Science, Kolkata, India

Nov. 2022 "Probing Realistic Water-2D Material Interfaces Via Combined Quantum & Classical Simulations", *Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks), AIChE 2022 Meeting*, Phoenix, Arizona, United States

Nov. 2022 "Predicting Defect Topologies in 2D Materials and their Effect on Molecular and Ionic Transport", *Colloquium, Center for Nanoscale Materials, Argonne National Laboratory*, Lemont, Illinois, United States (see https://www.anl.gov/cnm/cnm-colloquium-series)

Aug. 2022 "Predicting Defect Topologies in 2D Materials and their Effect on Molecular and Ionic Transport", Prof. Kumar V. Agrawal's group, *Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL),* Lausanne, Switzerland

Aug. 2022 "Predicting Defect Topologies in 2D Materials and their Effect on Molecular and Ionic Transport", Prof. Chih-Jen Shih's group, *Institute of Chemical and Bioengineering, ETH Zurich*, Zurich, Switzerland

Aug. 2022 "Artificial Intelligence for the Computational Design of Catalysts", Hindustan Petroleum Research Advisory Council Meeting, *HPCL Green R&D Centre, Bengaluru*, Karnataka, India

Mar. 2022 Panel Member in Researcher's RoundTable, American Chemical Society Spring 2022 India Satellite Meeting

Mar. 2022 "Learning to Predict the Probabilities and Formation Times of Arbitrary Nanopores in Graphene", Short-Term Course on Applications of MD and Machine Learning, *Department of Chemical Engineering, Indian Institute of Technology Madras*

Jan. 2022 "How Grain Boundaries and Interfacial Electrostatic Interactions Modulate Water Desalination Via Nanoporous Hexagonal Boron Nitride", Workshop on Thin Film Nanostructured Membranes for Gas Separation, Storage and Water Desalination*, Indian Institute of Science*, Bengaluru

Dec. 2021 "Modulating Water Slip Using Atomic-Scale Defects: Friction on Realistic Hexagonal Boron Nitride Surfaces", *Complex Fluids Symposium, India*

Sep. 2021 "Introduction to Boosting Algorithms in Machine Learning", Faculty Development Programme, *Department of Chemical Engineering, MVJ College of Engineering*

Jul. 2021 "Multi-Scale Simulations for Advancing Sustainable Hydrogen Production via Electrochemical Water Splitting", *Shell Research & Development Centre*, Bengaluru, India

Mar. 2021 "Multi-Scale Simulations for Advancing Sustainable Hydrogen Production via Electrochemical Water Splitting", *Department of Chemical Engineering, Indian Institute of Technology Gandhinagar*, Gujarat, India

Jan. 2021 "Combining Quantum and Classical Simulations for Modeling Interfaces", *Unilever India,* Bengaluru, India

Dec. 2020 "Wetting and Liquid-Solid Frictional Properties of 2D Materials", *Soft Matter Young Investigators e-Meet*, India

Nov. 2020 "Using Molecular Dynamics Simulations to Model Interfacial Properties of Nanomaterials", *Short-Term Course on Basic Principles of Density Functional Theory and Molecular Dynamics Simulations, Department of Chemical Engineering, Malaviya National Institute of Technology (MNIT)*, Jaipur, India

Nov. 2020 "Using Density Functional Theory to Model Heterogeneous Electrocatalysis", *Short-Term Course on Basic Principles of Density Functional Theory and Molecular Dynamics Simulations*, *Department of Chemical Engineering, Malaviya National Institute of Technology (MNIT)*, Jaipur, India

Oct. 2020 "Combining Quantum and Classical Simulations for Advancing Applications at the Water-Energy Nexus", *Department of Chemical Engineering, Indian Institute of Science, Bengaluru*, India

Oct. 2020 "Nanopores in and Nanofluidics on 2D Materials", *Center for Enhanced Nanofluidic Transport*, MIT, Cambridge, MA, United States

Jun. 2020 "Nanomaterials Simulations for Advancing Applications at the Water-Energy Nexus", *Microsoft Azure Global*, Seattle, WA, United States

Feb. 2020 "Modeling Thermodynamics and Kinetics at 2D Material Interfaces: Applications in Nanopore Formation and Electrocatalysis", *Department of Chemical Engineering, Indian Institute of Technology Madras*, Chennai, India

Jan. 2019 "Atomistic Modeling and Simulations of 2D Materials: Nanoporous Defects, Force-Field Development, and Wetting", *Department of Chemical Engineering, Indian Institute of Science*, Bengaluru, India

Jun. 2018 "Understanding the Surfactant-Induced Exfoliation and Dispersion of Carbon-Based Nanomaterials in Aqueous Solutions Using Molecular Dynamics Simulations", *Surfactants in Solution (SIS) 2018 Meeting*, University of Oklahoma, Norman, OK (on behalf of Blankschtein, D.)

Sep. 2017 "Understanding Interfacial Phenomena at 2D Material Interfaces using Atomistic Simulations: Chemical Vapor Deposition Growth, Wetting, and Liquid-Phase Exfoliation", *Department of Chemical Engineering, Indian Institute of Technology Delhi*, New Delhi, India

Jul. 2017 "Transport and Phase Behavior in Carbon Nanotube Nanofluidic Channels: Observing the Ionic Coulter Effect and Extreme Phase Transition Temperatures of Confined Water", *Telluride Science Workshop 2017,* Telluride, CO, United States (on behalf of Strano, M.S.)

Oct. 2015 "Transition Metal Dichalcogenides: Understanding Layer-Dependent Optoelectronic Properties and Vapor Synthesis", 2015 Annual Review Meeting, MIT-MTL Center for Graphene Devices and 2D Systems, MIT, Cambridge, MA, United States (on behalf of Strano, M. S.)

Contributed Talks and Posters

Nov. 2022 "Modeling the Combined Effects of Temperature, Pressure, and pH on Oxygen Evolution Thermodynamics and Kinetics", *AIChE 2022 Meeting*, Phoenix, Arizona, United States (with Martirez, J. M. P. and Carter, E. A.)

Sep. 2022 "Prediction of Accurate Enhancement Factors for Confined Water Flow in Boron Nitride Nanotubes", *International Conference on Chemical Engineering: Enabling Transition Towards a Sustainable Future*, Indian Institute of Technology Roorkee, Roorkee, India (presented by Kumar, S., who won the best oral presentation award for this talk)

Aug. 2022 "Combining Density Functional Theory and Kinetic Monte Carlo with Graph Theory and Machine Learning to Predict Nanopore Shapes in 2D Materials", *Psi-k 2022 Meeting,* Lausanne, Switzerland (with Sheshanarayana, R. and Bhowmik, S.)

Aug. 2022 "How Grain Boundaries and Interfacial Electrostatic Interactions Modulate Water Desalination via Nanoporous hBN", *American Chemical Society (ACS) Fall 2022 Meeting* (with Sharma, B. B.)

Aug. 2022 "Tailoring Nanoporous Graphene via Machine Learning: Predicting Probabilities and Formation Times of Arbitrary Nanopore Shapes", *American Chemical Society (ACS) Fall 2022 Meeting* (with Sheshanarayana, R.)

Mar. 2022 "Combined First-Principles and Classical Modeling of hBN-Water Interfaces: How Surface Roughness and Defects Modulate Wettability and Friction", *American Physical Society (APS) India Satellite March Meeting 2021* (presented by Verma, Ashutosh K.)

Dec. 2021 "Modulating Water Slip Using Vacancy Defects: Towards Realistic Modeling of Hexagonal Boron Nitride Surfaces", *Materials Research Society (MRS) Fall 2021 Meeting* (presented by Seal, A., who received a MRS travel award for this presentation)

Dec. 2021 "Enhancing Nanofluidic Transport using Atomic-Scale Defects: How Interfacial Interactions Modulate Water Slip on Boron Nitride Surfaces", *Theoretical Chemistry Symposium (TCS) 2021* (presented by Seal, A., who received a Phys. Chem. Chem. Phys. (PCCP) best poster prize for this poster)

Nov. 2021 "Understanding Water Slip on Defective Boron Nitride Surfaces: Combined Quantum and Classical Modeling of Solid–Liquid Friction", *American Institute of Chemical Engineers (AIChE) 2021 Meeting* (with Seal, A.)

Apr. 2021 "Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH: Different Chemistries Leading to Similar Overpotentials", *American Chemical Society (ACS) 2021 Spring Meeting* (with Martirez, J. M. P. and Carter, E. A.)

Apr. 2021 "Marcus-Theory Based Microkinetic Model for pH- and Potential-Dependent Water Splitting", *American Chemical Society (ACS) 2021 Spring Meeting* (with Carter, E. A.)

Apr. 2021 "Discovering Competing Electrocatalytic Mechanisms and their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways", *American Chemical Society (ACS) 2021 Spring Meeting* (with Carter, E. A.)

Apr. 2020 "A Mechanistic Model to Relate Thermodynamic and Kinetic Overpotentials: Elucidating the pH- and Temperature-Dependence of the Oxygen Evolution Reaction", *Materials Research Society (MRS) 2020 Spring Meeting and Exposition*, Phoenix, AZ (with Gopalakrishnan, S. G., Martirez, J. M. P., and Carter, E. A.) (canceled due to COVID-19)

Mar. 2020 "Revealing the Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH Using Hybrid Density Functional Theory: Different Chemistries Leading to Similar Overpotentials", *ACS Spring 2020 National Meeting and Exposition*, Philadelphia, PA (with Martirez, J. M. P. and Carter, E. A.) (canceled due to COVID-19)

Nov. 2019 "Modeling Thermodynamics and Kinetics at 2D Material Interfaces: Applications in Synthesis, Nanopore Formation, Wetting, and Catalysis", *AIChE 2019 Meeting*, Orlando, FL (with Strano, M. S., Strano, M. S., and Carter, E. A.)

Nov. 2019 "Advancing Nanomaterials for Energy and Water Applications using Atomistic and Quantum Chemical Simulations", Poster, *AIChE 2019 Meeting*, Orlando, FL

Nov. 2019 "Probing the Oxygen Evolution Reaction Efficacy of NiOOH (0001) and $(10\bar{1}0)$ Using Hybrid Density Functional Theory", Poster, *AIChE 2019 Meeting*, Orlando, FL (with Martirez, J. M. P. and Carter, E. A.)

Nov. 2018 "Development of Force Fields to Model Up-and-Coming Two-Dimensional Materials in Mechanical and Interfacial Applications", *AIChE 2018 Meeting,* Pittsburgh, PA (with Sresht, V., Padua, A. A. H., Strano, M. S., and Blankschtein, D.)

Nov. 2018 "Addressing the Isomer Cataloging Problem for Nanopores in Graphene and Other Two-Dimensional Materials", *AIChE 2018 Meeting,* Pittsburgh, PA (with Silmore, K., Swett, J., Robertson, A. W., Warner, J. H., Blankschtein, D. and Strano, M. S.)

Aug. 2018 "Ab Initio Molecular Dynamics and Lattice Dynamics-Based Force Field for Modeling Hexagonal Boron Nitride in Mechanical and Interfacial Applications", Poster, *256th ACS National Meeting and Exposition,* Boston, MA (with Strano, M. S. and Blankschtein, D.)

Aug. 2018 "Addressing the Isomer Cataloging Problem for Nanopores in Two-Dimensional Materials", *256th ACS National Meeting and Exposition,* Boston, MA (with Silmore, K., Swett, J., Blankschtein, D. and Strano, M. S.)

Aug. 2018 "Addressing the Isomer Cataloging Problem for Nanopores in Two-Dimensional Materials", Poster, *2018 CAMD Summer School on Electronic-Structure Theory,* Organized by Technical University of Denmark (DTU), Elsinore, Denmark (with Blankschtein, D. and Strano, M. S.)

Nov. 2017 "Nonpolar Wetting Behavior of Hexagonal Boron Nitride Offers Direct Evidence for the Existence of Dihedral Potentials", *Materials Research Society (MRS) 2017 Fall Meeting and Exposition*, Boston, MA (with Strano, M.S. and Blankschtein, D.)

Nov. 2017 "Cataloging Nanopore Isomers in Graphene Using Multiscale Atomistic Simulations", *Materials Research Society (MRS) 2017 Fall Meeting and Exposition*, Boston, MA (with Blankschtein, D. and Strano, M.S.)

Jun. 2017 "Quantitative Modeling of MoS_2-Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics", *Nanotech France 2017*, Paris, France (with Sresht, V., Bordes, E., Strano, M. S., Agilio, A. A. H., and Blankschtein, D.)

Dec. 2016	"Generalized Mechanistic Model for the Chemical Vapor Deposition of 2D Transition Metal Dichalcogenide Monolayers", *Materials Research Society (MRS) 2016 Fall Meeting and Exposition*, Boston, MA (with Warner, J. H., Blankschtein, D., and Strano, M. S.)
Dec. 2016	"Dominance of Dispersion Interactions and Entropy Over Electrostatics in Determining the Wettability and Friction of Two-Dimensional MoS_2 Surfaces", *Materials Research Society (MRS) 2016 Fall Meeting and Exposition*, Boston, MA (with Sresht, V., Padua, A.A.H., Strano, M.S., and Blankschtein, D.)
Nov. 2016	"Generalized Mechanistic Model for the Chemical Vapor Deposition of 2D Transition Metal Dichalcogenide Monolayers", AIChE 2016 Meeting, San Francisco, CA (with Warner, J. H., Blankschtein, D., and Strano, M. S.)
Nov. 2016	"The Role of Dispersion Interactions, Electrostatics, and Entropy in the Interfacial Behavior of MoS_2", *American Institute of Chemical Engineers (AIChE) 2016 Meeting*, San Francisco, CA (with Sresht, V., Padua, A.A.H., Strano, M.S., and Blankschtein, D.)
Aug. 2016	"Generalized Mechanistic Model for the Chemical Vapor Deposition of 2D Transition Metal Dichalcogenide Monolayers", 252nd ACS National Meeting & Exposition, Philadelphia, PA (with Warner, J. H., Blankschtein, D., and Strano, M. S.)
Jun. 2016	"Modeling the Interactions of Solvents with 2D MoS_2 Flakes: Predicting Contact Angles and Liquid-Phase Exfoliation Efficacy", Poster, Cabot Student Materials Research Forum, Billerica, MA (with Sresht, V., Bordes, E., Strano, M. S., Padua, A. A. H., and Blankschtein, D.)
Jun. 2016	"The Role of Dispersion Interactions, Electrostatics, and Entropy in the Interfacial Behavior of MoS_2", 90th ACS Colloid & Surface Science Symposium, Harvard University, Cambridge, MA (with Sresht, V., Padua, A.A.H., Strano, M.S., and Blankschtein, D.)
Dec. 2011	"Micro-Channel and Micro-Capillary Flows using the Extended Navier-Stokes Equation", 10th Indo-German Winter Academy, Surajkund, Delhi, India (one of the 2 students selected from IIT Delhi to attend a course on "Fluid Mechanics and Heat Transfer")

Teaching & Mentoring

Jan. Sem. 2023-pres.	*"Machine Learning for Materials and Molecules":* Instructor for postgraduate-level elective course; rated 4.47/5.0.
Jan. Sem. 2021-pres.	*"Introduction to Molecular Simulations":* Co-instructor for postgraduate-level elective course along with Prof. Sudeep Punnathanam at IISc; rated 4.4/5.0 and 4.73/5.0.
Aug. Sem. 2020-pres.	*"Engineering Mathematics"*: Co-instructor for postgraduate-level core course along with Prof. Prabhu Nott/Ganapathy Ayappa at IISc; rated 4.86/5.0, 4.56/5.0, and 4.75/5.0.
Fall 2017	*"How Do We Describe Fluid Flows?"*: 3-hour course for 15 high school students from 9-12th grade at MIT, as part of MIT Educational Studies Program's Splash initiative
Fall 2016	"*Chemical Engineering Thermodynamics"*: Teaching assistant for graduate-level core course by Prof. Daniel Blankschtein at MIT, conducted recitation sessions for 43 students, rated 6.3/7.0
Fall 2015	*"Fluids: Streams, Droplets, and Bubbles"*: 2-hour course for 12 high school students from 9-12th grade at MIT, as part of MIT Educational Studies Program's Splash initiative
Jan. Sem. 2013	*"Transport Phenomena"*: Teaching assistant for undergraduate-level core course by Prof. Sharad K. Gupta at IIT Delhi, conducted tutorial sessions for 40 students
2011 – 2012	Mentored a set of 6 incoming first year undergraduate students in Kumaon Hostel, IIT Delhi; adjudged best cross-hostel mentor

Industrial Experience

Mar. 2015 – May 2015 **Technical Consultant, Merck Sharp & Dohme (MSD), Ballydine, Ireland**
- Leading pharmaceutical manufacturer, $39.8 billion revenue (2016)
- Two one-month-long projects focused on: (i) quantitative analysis of plant data for **real-time improvement of the process yield** for proprietary drug manufacture at the Ballydine facility, and (ii) process troubleshooting to **de-bottleneck clogging** of filters in the **rotary compaction** of drug formulations

Jan. 2015 – Mar. 2015 **Technical Consultant, Cabot Corporation, Billerica MA, USA**
- Leading specialty chemicals manufacturer, $3.3 billion revenue (2012)
- Two one-month-long projects focused on: (i) understanding and improving the **dispersion of carbon black in rubber** for composite applications using modeling and experiments, and (ii) modeling and experimental studies of **water purification using activated carbon**: effect of pore size distribution on adsorption of dyes

May 2012 – Jul. 2012 **Summer Intern, Haldor Topsøe A/S, Lyngby, Denmark**
- Leading technology licensor for petrochemicals and fertilizers, $1 billion revenue (2015)
- Successfully setup **dynamic simulation** to model a Topsøe **hydro de-sulfurization plant** using 3 software packages: SIMSCI PRO/II, Dynsim, and HTRI

Selected Roles of Institutional Service

May. 2022 – present **President, Chemical Engineering Association, Department of Chemical Engineering, Indian Institute of Science**
Faculty president of the democratic, student-led association of the department responsible for organizing departmental events, including the annual symposium, as well as for maintaining the social media accounts of the department

Sep. 2020 – present **Convenor, Wellness Committee, Department of Chemical Engineering, Indian Institute of Science**
Convenor of the departmental committee responsible for maintaining mental wellness and inclusivity in the department

Sep. 2019 – Aug. 2020 **Member, Climate and Inclusion Committee, Department of Mechanical and Aerospace Engineering, Princeton University**
Member of a departmental committee overseeing efforts to enhance inclusivity in the department by promoting interactions between faculty, staff, and students

References

- **Professor Emily A. Carter**, *Gerhard R. Andlinger Professor in Energy and the Environment, Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics, Princeton University; Senior Strategic Advisor for Sustainability Science, Princeton Plasma Physics Laboratory*
  Relationship: *Postdoctoral Advisor*
  E-mail: eac@princeton.edu

- **Professor Daniel Blankschtein**, *Herman P. Meissner '29 Professor of Chemical Engineering, Massachusetts Institute of Technology*
  Relationship: *Doctoral Advisor*
  E-mail: dblank@mit.edu

- **Professor Michael S. Strano**, *Carbon P. Dubbs Professor of Chemical Engineering, Massachusetts Institute of Technology*
  Relationship: *Doctoral Advisor*

E-mail: srgoffice@mit.edu

- **Professor Shantanu Roy**, *Institute Chair Professor of Chemical Engineering, Indian Institute of Technology Delhi*
  Relationship: *B.Tech. Thesis Advisor*
  E-mail: roys@chemical.iitd.ac.in