Ritesh Kumar

CONTACT INFORMATION	Pritzker School of Molecular Engineering, University of Chicago
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Personal website: https://ritesh001.github.io/ai4en/

EDUCATION

Ph.D. in Materials Science
August 2017 – January 2022

Indian Institute of Science, Bangalore, India

Advisor: Prof. Abhishek Singh

Thesis: Rational design of efficient catalysts using first-principles and machine learning

M.S. in Chemical Science
July 2015 – July 2017

Indian Institute of Science, Bangalore, India

Advisor: Prof. Abhishek Singh

Thesis: Earth-abundant electro- and photocatalysts as energy alternatives: An *ab initio* study

B.Sc. in Chemistry (Honors)
July 2012 – April 2015

Sri Venkateswara College (University of Delhi), New Delhi, India

First Division

PROFESSIONAL EXPERIENCE

University of Chicago, Pritzker School of Molecular Engineering
January 2022 – Present

Eric & Wendy Schmidt AI in Science Fellow and Postdoctoral Scholar, Chibueze Amanchukwu's Lab

- Developed custom machine learning (ML) techniques for electrolyte discovery for next-generation batteries and built largest liquid electrolyte databases
- Enhanced Bayesian optimization technique for real-world discovery of electrolytes in data-scarce and noisy-label settings
- Developed generative AI and unsupervised frameworks for electrolyte discovery to overcome selection bias associated with existing exploration
- Currently coupling my data-driven framework with automated high-throughput battery assembly and testing platform for accelerated experimental validation
- Elucidated atomistic insights into experimental electrolyte performance for next-generation batteries using *ab initio* molecular dynamics (MD)
- Formulated inexpensive computational descriptors through MD simulations to explain aprotic electrolyte effects in key industrial reactions (CO_2/CO reduction)
- Co-developed a software `AtomBridge` for automated conversion of STEM images to crystal structures using LLMs and computer vision: https://github.com/dpalmer-anl/AtomBridge
- Led development of a software `curAItor-agent` for automated scientific data extraction using LLMs and AI agents: https://github.com/ritesh001/curaitor-agent

Indian Institute of Science, Materials Research Centre
August 2016 – January 2022

Graduate Research Student (Ph.D. and Master's), Abhishek Singh's Lab

- Developed robust design principles using quantum mechanical density functional theory (DFT) for efficient heterogeneous catalysts in key industrial reactions such as solar hydrogen production, ammonia synthesis, and artificial photosynthesis
- Demonstrated atomistic origin of efficient catalysts for fuel cells, CO_2 electroreduction, hydrogen generation among others, in collaboration with experimentalists
- Designed novel nanomaterials for electronic and spintronic applications based on DFT modeling
- Introduced governing principles for nanomaterial stability in photocatalysis using interpretable ML for the first time, contributing to a publicly accessible database at https://anant.mrc.iisc.ac.in/apps/2D

Indian Institute of Technology, Ropar, Department of Chemistry
May 2014 – July 2014

Summer Undergraduate Research Fellow, Narinder Singh's Lab

- Designed and analyzed supramolecular organic-inorganic hybrid nanoparticles using flourescence spectroscopy and cyclic voltammetry for chemical sensors

PUBLICATIONS
(† denotes equal
contribution)

22. P. Ma[†], **R. Kumar**[†], K.-H. Wang, C. V. Amanchukwu, "Active learning accelerates electrolyte solvent screening for anode-free lithium metal batteries." *Nat. Commun.* 16, 8396 (2025).

21. H. Fejzic, **R. Kumar**, R. J. Gomes, L. He, T. J. Houser, J. Kim, N. Molten, C. V. Amanchukwu. "Water Clustering Modulates Activity and Enables Hydrogenated Product Formation during Carbon Monoxide Electroreduction in Aprotic Media." *J. Am. Chem. Soc.* 147, 18445-18459 (2025).

20. **R. Kumar**, M. C. Vu, P. Ma, C. V. Amanchukwu. "Electrolytomics: A Unified Big Data Approach for Electrolyte Design and Discovery." *Chem. Mater.* 37, 2720-2734 (2025).

19. R. J. Gomes, **R. Kumar**, H. Fejzic, B. Sarkar, I. Roy, C. V. Amanchukwu. "Modulating Water Hydrogen Bonding within a Nonaqueous Environment Controls its Reactivity in Electrochemical Transformations" *Nat. Catal.* 7, 689-701 (2024).

18. E. S. Doyle, P. Mirmira, P. Ma, M. C. Vu, T. Hixson-Wells, **R. Kumar**, C. V. Amanchukwu. "Phase Morphology Dependence of Ionic Conductivity and Oxidative Stability in Fluorinated Ether Solid-State Electrolytes." *Chem. Mater.* 36, 5063-5076 (2024).

17. P. Ma, **R. Kumar**, M. C. Vu, K.-H. Wang, P. Mirmira, C. V. Amanchuwku. "Fluorination promotes lithium salt dissolution in borate esters for lithium metal batteries." *J. Mater. Chem. A* 12, 2479-2490 (2024).

16. P. V. Sarma[†], R. Nadarajan[†], **R. Kumar**, R. M. Patinharayil, N. Biju, S. Narayanan, G. Gao, C. S. Tiwary, M. Thalakulam, R. Kini, A. K. Singh, P. M. Ajayan, M. Shaijumon. "Growth of Highly Crystalline Ultrathin Two-Dimensional Selenene." *2D Mater.* 9, 045004 (2022).

15. R. Das, S. Sarkar, **R. Kumar**, S. D. Ramarao, A. Cherevotan, M. Jasil, C. P. Vinod, A. K. Singh, S. C. Peter. "Noble-Metal-Free Heterojunction Photocatalyst for Selective CO_2 Reduction to Methane upon Induced Strain Relaxation." *ACS Catal.* 12, 687-697 (2022).

14. L. Sharma[†], N. K. Katiyar[†], A. Parui[†], R. Das, **R. Kumar**, C. S. Tiwary, A. K. Singh, Aditi Halder, Krishanu Biswas. "Low-Cost High Entropy Alloy (HEA) for High-Efficiency Oxygen Evolution Reaction (OER)." *Nano Res.* 15, 4799-4806 (2022).

13. **R. Kumar**, and A. K. Singh. "Chemical Hardness-Driven Interpretable Machine Learning for Rapid Search of Photocatalysts." *NPJ Comput. Mater.* 7, 1-13 (2021).

12. S. Agarwal, **R. Kumar**, R. Arya, and A. K. Singh. "Rational Design of Single-Atom Catalysts for Enhanced Electrocatalytic Nitrogen Reduction Reaction." *J. Phys. Chem. C* 125, 12585–12593 (2021).

11. **R. Kumar**, and A. K. Singh. "Electronic Structure Based Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction." *ChemCatChem* 12, 5456–5464 (2020).

10. R. Nandan, R. Hemam, **R. Kumar**, A. K. Singh, C. Srivastava, and K. K. Nanda. "Inner Sphere Electron Transfer Promotion on Homogeneously Dispersed $Fe-N_X$ Centres for Energy Efficient Oxygen Reduction Reaction." *ACS Appl. Mater. Interfaces* 12, 36026–36039 (2020).

9. P. Sarma, T. V. Vineesh, **R. Kumar**, V. Sreepal, A. K. Singh, and M. Shaijumon. "Nanostructured Tungsten Oxysulfide as an Efficient Electrocatalyst for Hydrogen Evolution Reaction." *ACS Catal.* 10, 6753–6762 (2020).

8. K. Urs[†], N. K. Katiyar[†], **R. Kumar**, K. Bishwas, A. K. Singh, C. S. Tiwary, and V. B. Kamble. "Multi-component (Ag-Au-Cu-Pd-Pt) Alloy Nanoparticles Decorated p-type 2D-Molybdenum Disulphide (MoS_2) for Enhanced Hydrogen Sensing" *Nanoscale* 12, 11830–11841 (2020).

7. N. K. Katiyar[†], S. Nellaiappan[†], **R. Kumar**[†], K. D. Malviya, K. G. Pradeep, A. K. Singh, S. Sharma, C. S. Tiwary, and K. Bishwas. "Formic Acid and Methanol Electro-oxidation and Counter Hydrogen Production Using Nano High Entropy Catalyst." *Mater. Today Ener.* 16, 100393 (2020).

6. S. Nellaiappan[†], N. K. Katiyar[†], **R. Kumar**[†], A. Parui, K. D. Malviya, K. G. Pradeep, A. K. Singh, S. Sharma, C. S. Tiwary, and K. Bishwas. "High-Entropy Alloys as Catalysts for the CO_2 and CO Reduction Reactions: Experimental Realization." *ACS Catal.* 10, 3658–3663 (2020).

5. S. Nellaiappan, **R. Kumar**, S. C., S Irusta, J. A. Hachtel, J. C. Idrobo, A. K. Singh, C. S. Tiwary, and S. Sharma. "Electroreduction of Carbon Dioxide into Selective Hydrocarbon at Low Overpotential using Isomorphic Atomic Substitution in Copper Oxide." *ACS Sustainable Chem. Eng* 8, 179–189 (2020).

4. R. K. Barik, **R. Kumar**, and A. K. Singh. "Topological Phases in Hydrogenated Group 13 Monolayers." *J. Phys. Chem. C* 123, 25985–25990 (2019).

3. **R. Kumar**, D. Das, E Munoz, and A. K. Singh. "Critical Sublattice Symmetry Breaking: A Universal Criterion for Dirac Cone Splitting." *J. Phys. Chem. C* 123, 23082–23088 (2019).

2. A. P. Balan[†], S. Radhakrishnan[†], **R. Kumar**, R. Neupane, S. K. Sinha, L. Deng, C. A. de los Reyes, A. Apte, B. M. Rao, M. Paulose, R. Vajtai, C. W. Chu, G. Costin, A. A. Martí, O. K. Varghese, A. K. Singh, C. S. Tiwary, M. R. Anantharaman, and P. M. Ajayan, "A Non-van der Waals Two-Dimensional Material from Natural Titanium Mineral Ore Ilmenite." *Chem. Mater.* 30, 5923–5931 (2018).

1. **R. Kumar**, D. Das, and A. K. Singh, "C_2N/WS_2 Van der Waals Type-II Heterostructure as a Promising Water Splitting Photocatalyst." *J. Catal.* 359, 143–150 (2018).

CONFERENCE PROCEEDINGS

1. S. A. Eshiemogie, **R. Kumar**, C. V. Amanchukwu, "Data Preprocessing and Machine Learning Modelling for Battery Electrolyte Discovery." *2024 Int. Conf. Sci., Eng. Bus. Driv. Sustain. Dev. Goals (SEB4SDG)* (2024) (https://doi.org/10.1109/seb4sdg60871.2024.10630085).

PREPRINTS/ MANUSCRIPTS SUBMITTED

3. **R. Kumar**[†], K.-H. Wang[†], C. V. Amanchukwu, "Using Electrolyte Solvent Embeddings to Guide Battery Electrolyte Discovery." *ChemRxiv* (2025) (https://doi.org/10.26434/chemrxiv-2025-7nnbl).

2. **R. Kumar**, K.-H. Wang, Z. Umlauf, C. V. Amanchukwu, "ElectroNN: Interpretable Deep Learning Framework for Accurate Property Prediction and Generation of Electrolytes.".

1. J. Kim, K.-H. Wang, **R. Kumar**, P. Ma, C. V. Amanchukwu, "Generative Electrolyte Solvent and Formulation Discovery.".

AWARDS AND HONORS

8. Named 2025 Rising Stars in Soft and Biological Matter, co-sponsored by University of Chicago & University of California San Diego
December 2025

7. Selected for the Future Faculty Mentoring Program by American Institute of Chemical Engineering (AIChE)
October 2025

6. CAS Future Leader Top 100 Award by American Chemical Society (ACS)
March 2025

5. Eric & Wendy Schmidt AI in Science Postdoctoral Fellow (Salary: $80,000 per annum)
January 2023 – January 2026

4. Selected for Oxford Research Software Engineering (OxRSE) Workshop at University of Oxford, UK (travel grant; ~$3000)
June 2024 & September 2025

3. All India Rank 38 in IIT-Joint Admission test for Master's (IIT-JAM) Examination (Scholarship: ₹16,000 per month during Master's at Indian Institute of Science)
February 2015

2. IASc-INSA-NASI Summer Research Fellowship (organized by all three national academies of India) (Stipend: ₹8,000 per month)
May 2014 – July 2014

1. Central Sector Scheme of Scholarship for College and University Students (Scholarship: ₹10,000 per annum)
2012 – 2015

1. All-India Rank 54 in 2nd Nationwide Interactive Math Olympiad
November 2007

GRANTS

AI+Science Research Initiative Fund
Funding agency: Data Science Institute, University of Chicago, IL
Project title: Self-driving battery lab to accelerate scientific discovery
Role: PI
Amount: $10,000
January 2024

University of Chicago Women's Board Grant Fund
Funding agency: University of Chicago Women's Board
Project title: Artificial intelligence-guided autonomous high-throughput battery manufacturing platform to accelerate scientific discoveries
Role: Co-I
Amount: $50,000
June 2023

ORAL PRESENTATIONS	13. "Accelerating next generation battery materials discovery using active learning." *2025 Rising Stars in Soft and Biological Matter*, (Virtual; **Invited by Prof. Shrayesh Patel**)	December 2025
	12. "Accelerating liquid electrolyte discovery for next-generation batteries using data-driven techniques." *ZERO Institute Seminar*, University of Oxford, OX, UK (**Invited by Prof. David Howey**)	September 2025
	11. "Accelerating electrolyte discovery for next-generation batteries." *Prof. Venkatasubramanian Viswanathan's Lab Group Meeting*, University of Michigan, Ann Arbor, MI (**Invited by Prof. Venkatasubramanian Viswanathan**)	August 2025
	10. "Accelerating electrolyte discovery for batteries." *2025 MRS Spring Meeting and Exhibit*, Seattle, WA	April 2025
	9. "Powering Next-Generation Batteries through Data Science in Synergy with Simulations and Experiments." *Faculty Candidates in CoMSEF, 2024 AIChE Annual Meeting*, San Diego, CA	October 2024
	8. "Data-Driven Accelerated Discovery of Novel Battery Materials." *Frontiers of Machine Learning on Materials Discovery Symposium, MS&T24 Technical Meeting and Exhibition*, Pittsburgh, PA (**Invited by Dr. Rinkle Juneja**)	October 2024
	7. "Accelerating realization of next-generation batteries through data-driven techniques." *Chemistry Colloquium*, Illinois Institute of Technology, Chicago, IL (**Invited by Prof. Yuanbing Mao**)	September 2024
	6. "Graph neural networks for electrolytes." *2024 University of Chicago Schmidt AI in Science Postdoctoral Fellows Retreat*, North Utica, IL	September 2024
	5. "AI-driven discovery of efficient materials for next-generation batteries." *Computational Materials Science and Engineering Gordon Research Seminar (GRS)*, Sunday River, ME (**Invited by Prof. Aditya Nandy**)	July 2024
	4. "Realizing next-generation batteries through AI and automation." *2024 AI+Science Schmidt Fellow Speaker Series*, University of Chicago, IL (**Invited by Prof. Madeleine Torcasso**)	April 2024
	3. "A Big Data Approach to Rational Design and Discovery of Electrolytes." *243rd ECS Meeting*, Boston, MA	May 2023
	2. "Chemical Hardness-Driven Interpretable Machine Learning for Rapid Search of Photocatalysts." *2021 MRS Fall Meeting and Exhibit* (Virtual)	December 2021
	1. "Electronic Structure Based Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction." *2021 MRS Spring Meeting and Exhibit* (Virtual)	April 2021
POSTER PRESENTATIONS	10. "AI-driven realization of next-generation batteries." *AI+Science Summer School 2025*, Paris, France	July 2025
	9. "Accelerating Sustainable Energy Solutions through Data Science and Simulations in Synergy with Experiments." *Meet the Faculty and Post-Doc Candidates Poster Session, 2024 AIChE Annual Meeting*, San Diego, CA	October 2024
	8. "Tackling Energy Conversion Challenges through Simulations in Synergy with Experiments." *Poster Session: Computational Molecular Science and Engineering Forum, 2024 AIChE Annual Meeting*, San Diego, CA	October 2024

7. "*In Silico* Materials Design and Discovery for Electrocatalysis and Energy Storage." Early career poster at *AI for Multidisciplinary Exploration and Discovery (AIMED) Workshop on Heterogeneous Catalysis*, Big Ten Conference Center, Rosemont, IL (**Invited by Prof. Hongliang Xin**)

October 2024

6. "Achieving Sustainability through *In Silico* Materials Design and Discovery." *Computational Materials Science and Engineering Gordon Research Conference (GRC)*, Sunday River, ME

July 2024

5. "How can AI Power Next-Generation Batteries?" *2023 University of Chicago Schmidt AI in Science Postdoctoral Fellows Retreat*, Lake Geneva, WI

September 2023

4. "How can AI Power Next-Generation Batteries?" *AI in Science Postdoctoral Fellowship 2023 Inaugural Convening*, University of Toronto, Canada

August 2023

3. "Artificial Intelligence Powering Next-Generation Batteries." *University of Chicago and Caltech Conference on AI+Science*, University of Chicago, IL

March 2023

2. "C_2N/WS_2 Van der Waals Type-II Heterostructure as a Promising Water Splitting Photocatalyst." *Operando Surface Science – Atomistic Insights into Electrified Solid/liquid Interfaces Seminar*, Bad Honnef, Germany

December 2019

1. "C_2N/WS_2 Van der Waals Type-II Heterostructure as a Promising Water Splitting Photocatalyst." *Modelling and Simulations of Materials for Energy and Environment School*, Jawaharlal Nehru Centre for Advance Scientific Research, Bangalore, India

December 2018

TEACHING EXPERIENCE

University of Chicago
2. Guest lecturer, *Thermodynamics of phase equilibria*
1. Guest lecturer, *Energy conversion and storage devices*
(Additionally served as a panel judge for student final presentations, providing critical feedback and assessments)

October 2025
March 2024

Indian Institute of Science
2. Teaching assistant, *Computational modeling of materials*
(Developed and taught new hands-on course content, including comprehensive tutorials tailored to enhance practical learning, held weekly discussions, and graded exams)
1. Teaching assistant, *Quantum chemistry and group theory*
(Taught lectures, graded exams, and conducted exam performance review sessions)

January – May 2020

August – December 2019

MENTORING EXPERIENCE

University of Chicago
Undergraduates: 1. Arnav Brahmasandra (Computer Science)
2. Zoe Umlauf (Computer Science)
3. Leyou Gessessew (Data Science; Wellesley College; *AI+Science Research Experience for Undergraduates (REU) Summer Lab Program*)
Master's: 4. Tarun Arora (Computer Science)
5. Jaemin Kim (Chemistry): Co-authored one manuscript and one under review
Ph.D.: 6. Emily Doyle: Co-authored one publication

January 2023 – March 2024
January 2025 – June 2025
June – August 2025

June 2023 – March 2024
May 2023 – September 2025
May 2023 – present

RENEU program hosted by University of Chicago (remote)
Undergraduate: 1. Stanley Eshiemogie (University of Benin, Nigeria): Mentored a 10-week project on developing deep learning models for electrolyte property prediction, resulting in a co-authored article in the IEEE conference proceedings (current position: Ph.D. student at UChicago)

June 2023 – August 2023

Indian Institute of Science
Undergraduate: 1. Rakesh Arya (Chemistry major): Co-authored one publication and mentoring contributed to an undergraduate thesis
Master's: 2. Arko Parui: Co-authored 2 publications and mentoring contributed to a master's thesis
3. Pooja Gakhad: Mentoring contributed to a master's thesis

Janaury 2018 – January 2019

August 2018 – July 2019

December 2020 – July 2021

PROFESSIONAL DEVELOPMENT	**2025 Oxford Research Software Engineering Workshop** *Location*: Doctoral Training Centre, University of Oxford, UK *Description*: Led a team of 7 members to develop a graphical interface `curAItor-agent` for autonomous scientific data extraction using LLMs and AI agents (open-sourced at https://github.com/mmore500/curaitor) *Travel fund:* Schmidt Sciences, New York, NY	September 2025
	2025 LLM Hackathon for Applications in Materials Science & Chemistry *Location*: Virtual *Description*: Co-developed a tool `AtomBridge` for scientific automated conversion of STEM images to crystal structures using LLMs and computer vision (open-sourced at https://github.com/dpalmer-anl/AtomBridge) *Award:* 2025 Visionary Award	September 2025
	Teaching in the Generative AI Landscape *Location*: University of Chicago, IL *Description:* Workshop on enhanced student learning strategies using generative AI	September 2024
	2024 Oxford Research Software Engineering Workshop *Location*: Doctoral Training Centre, University of Oxford, UK *Description*: Co-developed a graphical interface `curAItor` for scientific data extraction using LLMs (open-sourced at https://github.com/mmore500/curaitor) *Travel fund:* Schmidt Sciences, New York, NY	June 2024
	Academic Job Market Summer Camp *Location*: University of Chicago, IL *Description*: Workshop on writing effective application materials for faculty jobs	July 2023
PROFESSIONAL MEMBERSHIPS	American Institute of Chemical Engineers (AIChE) American Institute of Chemical Engineers (AIChE) The Electrochemical Society (ECS) Materials Research Society (MRS)	2025 – 2026 2024 – 2025 2023 – 2024 2020 – 2022
COMPUTING ALLOCATIONS	**National Science Foundation (NSF) ACCESS** *Role:* PI *Award (system & CPU/GPU hours & estimated value):* 2. Discovery allocation (Purdue Anvil AI & GPU: 1000 & $234.51) 1. Discovery allocation (Purdue Anvil & CPU: 625,000 & $2,600.00)	 October 2025 October 2024
	Research Computing Center, University of Chicago *Role:* PI *Award (system & CPU hours):* 3. Research allocation (Midway & 100,000) 2. Research allocation (Midway & 100,000) 1. Startup allocation (Midway & 10,000)	 October 2025 October 2024 August 2024
SERVICE & OUTREACH	16. Reviewer, *Nature Communications* (1), *ACS Applied Energy Materials* (1), *Digital Discovery* (4), *Journal of Open Source Software* (2), and *Catalysts* (1)	November 2024 – October 2025
	15. Organizer, *2024-25 AI+Science Schmidt Fellows Speaker Series*, University of Chicago, IL (Revised second edition of the seminar series based on feedback and invited Prof. Aaron Dinner from University of Chicago Chemistry, Prof. Claire Donnat from University of Chicago Statistics, and Prof. Chibueze Amanchukwu)	October 2024 – May 2025
	14. Session chair, *Frontiers of Machine Learning on Materials Discovery Symposium, MS&T24 Technical Meeting and Exhibitio*, Pittsburgh, PA (**Invited by Dr. Rinkle Juneja**)	October 2024
	13. Discussion leader, *Computational Materials Science and Engineering Gordon Research Seminar*, Sunday River, ME (**Invited by Prof. Aditya Nandy**)	July 2024

12. Session chair and organizer, *2024 AI+Science Summer School*, University of Chicago, IL (Co-developed program for an multidisciplinary summer school for undergraduate and graduate students and postdocs, reviewed their applications, and invited Prof. Pedram Hassanzadeh from University of Chicago Geophysics, Dr. Zachary Ulissi from Meta FAIR, Dr. Muratahan Aykol from Google DeepMind) — July 2024

11. Reviewer, *US DOE Office of Science Graduate Student Research (SCGSR) program's 2024 Solicitation 1* (reviewed 3 Ph.D. student proposals) — June 2024

10. Organizer, *2024 AI+Science Hackathon*, University of Chicago, IL (Co-created hackathon, fostering a collaborative problem-solving in scientific AI) — May 2024

9. Resource person, "Introduction to use of AI in teaching and learning." *Workshop on AI for teaching & learning*, Sri Venkateswara College, India (Presented 3 hours-long tutorial for workshop attended by >80 faculties) (Virtual, **Invited by Prof. Sharda Pasricha**) — May 2024

8. Technical blogger, "Unlocking the Potential of Lithium Batteries with New Electrolyte Solutions", Data Science Institute Insights, University of Chicago, IL (*https://datascience.uchicago.edu/insights/unlocking-the-potential-of-lithium-batteries-with-new-electrolyte-solutions/*) — February 2024

7. Moderator and organizer, *2023-24 AI+Science Schmidt Fellows Speaker Series*, University of Chicago, IL (Co-developed and moderated a seminar series, enhancing academic dialogue and networking among scholars and invited Dr. Logan Ward from Argonne National Laboratory) — October 2023 – May 2024

6. Discussion leader, *Postdoc Program Leaders Community Forum*, organized by National Postdoctoral Association (NPA) (Virtual, **Invited by Thomas P. Kimbis**) — August 2023

5. Moderator, *2023 AI+Science Summer School*, University of Chicago, IL — July 2023

4. Judge, *Students Slam Contest at 243rd ECS Meeting*, Boston, MA (**Invited by Prof. Lin Ma and Prof. Betar Gallant**) — May 2023

3. Demonstration volunteer, Battery fabrication demonstration at *Science Works*, Museum of Science and Industry, Chicago, IL — October 2022

2. Incharge, High-performance computing facilities (hardware & software) at Materials Research Centre, Indian Institute of Science, Bangalore — August 2018 – July 2020

1. Demonstration volunteer, *2018 IISc Open day*, Institute of Science, Bangalore — March 2018