Kiran **Vaddi**

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Benson Hall, University of Washington, Seattle, WA, USA

Education

May 2021 – August 2017 | **University at Buffalo, The State University of New York, Buffalo, NY, USA**
PhD in Materials Science and Engineering
Thesis : Representations for data-driven material discovery

June 2017 – June 2016 | **Indian Institute of Technology Madras, Chennai, TN, India**
M.Tech in Thermal Engineering
Thesis : Luminescent solar concentrators using high-contrast gratings

June 2016 – June 2012 | **Indian Institute of Technology Madras, Chennai, TN, India**
Major : B.Tech in Mechanical Engineering
Minor : Industrial Engineering

Professional Experience

June 2021 – Present | **University of Washington, Seattle, WA**
Data Science Postdoctoral Fellow, Department of Chemical Engineering
- Developed closed-loop material acceleration platforms emphasizing learning faithful data representations of spectroscopy, and scattering characterizations of polymer, colloid, and soft-matter systems.

June 2017 – June 2021 | **University at Buffalo, Buffalo, NY, USA**
Graduate Research Assistant
- Developed physics-based models for cyclic voltammetry, phase diagrams of polymer blends, and data-driven models for structure-property relations for catalysis and organic photovoltaics.

June 2016 – June 2017 | **Industrial Interships**
- **Caterpillar India Pvt.Ltd :** Finite element-based modeling of thermal stresses in automotive engine components (gaskets)
- **Continental Automotive Components India Pvt.Ltd :** Finite element-based dynamic (vibration and failure) analysis of automotive engine components

June 2016 – June 2017 | **Indian Institute of Technology Madras, Chennai, TN, India**
Undergradte Research
- Construction of constitutive models for diffusion-induced deformation of photopolymer under selective irradiation

Teaching Experience

January 2023 – March 2023 | **Primary Instructor, Special Topics in Chemical Engineering : Design of Experiments**
CHEM E 599 B, Winter quarter, **Evaluation 4.2/5**
- Designed and delivered a graduate-level course on the design of experiments with applications in materials science and chemical engineering.

March 2022 – June 2022 | **CAPSTONE DIRECT project**
CHEME / CHEM / MSE 547 : Molecular Data Science Capstone
- Mentored five graduate students from the Department of Materials Science toward their final project titled “The infinite space of spectroscopy measurements” at the University of Washington.

Publications & Pre-prints

Vaddi, K., Chiang, H. T., Pozzo, L. D *“Autonomous Phase Mapping of Gold Nanoparticles Synthesis with Differentiable Models of Spectral Shape”*
ChemRxiv, 2025, DOI : 10.26434/chemrxiv-2025-zktwx (**Corresponding Author**)

HT Chiang, Z Zhang, **K Vaddi**, A Tezcan, L Pozzo *"Efficient Analysis of Small-Angle Scattering Curves for Large Biomolecular Assemblies Using Monte Carlo Methods"*
ChemRxiv, 2025, DOI : 10.26434/chemrxiv-2025-68833

K Vaddi, HT Chiang, LD Pozzo *"Autonomous Phase Mapping of Gold Nanoparticles Synthesis with Differentiable Models of Spectral Shape"*
ChemRxiv, 2025, DOI : 10.26434/chemrxiv-2025-zktwx

K Li, **K Vaddi**, S Seifert, J Mata, LD Pozzo *"Self-assembly of a Triblock Copolymer in the Presence of a Rigid Conjugated Polyelectrolyte"*
Macromolecules 57.24 (2024) : 11717-11726.

Chiang, Huat Thart, **Kiran Vaddi**, and Lilo D. Pozzo. *"Data-Driven Exploration of Silver Nanoplate Formation in Multidimensional Chemical Design Spaces"*
Digital Discovery, 2024, DOI : 10.1039/D4DD00211C

Vaddi, Kiran, Karen Li, and Lilo D. Pozzo. *"Metric geometry tools for automatic structure phase map generation."*
Digital Discovery, 2023, DOI : 10.1039/D3DD00105A (Corresponding Author)

Politi, M., Baum, F., **Vaddi, K.**, Vasquez, J., Antonio, E., Bishop, B. P., ..., and Pozzo, L. D. *"High-Throughput Workflow for the Synthesis of CdSe Nanocrystals Using a Sonochemical Materials Acceleration Platform."*
Digital Discovery, 2023, 2, 1042-1057 (Editor's Choice 2023)

Vaddi, K., Liu, H., Pokuri, B. S. S., Ganapathysubramanian, B., and Wodo, O. (2023) *"Construction and high throughput exploration of phase diagrams of multi-component organic blends"*
Computational Materials Science 216 (2023) : 111829.

Vaddi, Kiran, Huat Thart Chiang, Lilo D. Pozzo *"Autonomous retrosynthesis of gold nanoparticles via spectral shape matching"*
Digital Discovery 1.4 (2022) : 502-510 (Editor's Choice 2022, Corresponding Author)

Lachowski, K. J., **Vaddi, K.**, Naser, N. Y., Baneyx, F., Pozzo, L. D. *"Multivariate Analysis of Peptide-Driven Nucleation and Growth of Au Nanoparticles"*
Digital Discovery 1.4 (2022) : 427-439

Vaddi, Kiran, Olga Wodo *"Active knowledge extraction from cyclic voltammetry"*
Energies 15.13 (2022) : 4575

Elikkottil, A., **Vaddi, K.**, Reddy, K. S., Pesala, B. *"Reduction of Escape Cone Losses in Luminescent Solar Concentrators Using High-Contrast Gratings."*
In Advances in Energy Research, Vol. 1 (pp. 37-43). Springer, Singapore, 2020

Vaddi, Kiran, and Olga Wodo. *"Metric Learning for High-Throughput Combinatorial Data Sets."*
ACS Combinatorial Science 21.11 (2019) : 726-735 (Corresponding Author)

Grant Proposals

June 2022 – June 2025 | **AI-Accelerated Optimization of Self-Assembled Organic Mixed Ionic-Electronic Conductors (OMIEC)**
DOE- Basic Energy Sciences-Neutron Scattering (Awarded DE-SC0019911)
- Contributed to this PI-led Energy grant on building AI-driven workflows understanding a novel class of OMIEC materials based on conjugated polymer blends from the Department of Energy (30%).

June 2023 | **Accelerating the structure-based material retrosynthesis using shape representations**
2022 Acceleration Consortium Project Theme : Machine learning algorithms for synthesis protocols
- Led a proposal to advance self-driving laboratories for soft-matter systems as part of the University of Toronto's Acceleration Consortium, which received an honorable mention (80%).

Awards

February 2025 | **Future Investigator Travel Award**
American Physical Society Division of Soft Materials

September 2024	**Outstanding Reviewer Award** Royal Society of Chemistry Digital Discovery Journal
December 2023	**Best Poster Award** Materials Research Society Fall Meeting-Symposium on Data Science
March 2023	**Data Science Conference Travel Award** eScience Institute, University of Washington, Seattle, WA
June 2021	**UW Data Science Postdoctoral Fellowship** eScience Institute, University of Washington, Seattle, WA
August 2013	**Outstanding Undergraduate Service Award** National Service Scheme, Indian Institute of Technology Madras

Invited talks

December 2023 Invited Panelist	**The Kavli Foundation Frontiers of Materials, Boston, MA, USA** Symposium X - How to Build a Self-Driving Lab Keith A. Brown, John Dunlap, Robert Epps, Jason Hattrick-Simpers, **Kiran Vaddi**
December 2023 Invited talk	**Materials Research Society, Boston, MA, USA** A Tutorial on Functional Data Analysis for High-Throughput Experiments **Kiran Vaddi**
October 2023 Invited talk	**UW Data Science Seminar, Seattle, WA, USA** Functional data analysis tools for autonomous experimentation **Kiran Vaddi**
August 2023 Invited talk	**American Chemical Society Fall Meeting, San Francisco, CA, USA** Cold, warm, warmer, hot! Impact of distance metrics on autonomous experimentation **Kiran Vaddi**, Kacper Lachowski, Huat T Chiang, Karen Li, Lilo D. Pozzo
January 2020 Invited talk	**IEEE Rochester Section Chapter, Rochester, NY, USA** Function Space Data Representation of Temporal Signals for Machine Learning **Kiran Vaddi**

Select Conference Presentations & Posters

August 2024 Contributed talk	**American Chemical Society Fall Meeting, Denver, CO, USA** Understanding Design Rules of Colloidal Self-Assembly Using Autonomous Phase Mapping **Kiran Vaddi**, Huat T Chiang, Lilo D. Pozzo
April 2024 Contributed talk	**Materials Research Society Spring Meeting, Seattle, WA, USA** High-Throughput Structural Investigation of Block Copolymer and Conjugated Polymer Co-Assemblies **Kiran Vaddi**, Karen Li, Lilo D. Pozzo
December 2023 Poster	**Materials Research Society Fall Meeting, Boston, MA, USA** Function Space Representations for Complex Material Workflows **Kiran Vaddi** (Best poster award)
March 2023 Contributed talk	**American Physics Society March Meeting, Las Vegas, NV, USA** Metric geometry tools for automatic structure phase map generation **Kiran Vaddi**, Karen Li, Lilo D. Pozzo
August 2022 Poster	**Gordon Research Conference on Computational Materials Sciences, Newry, ME, USA** Shape-based data representations for experimental spectra **Kiran Vaddi**, Huat T Chiang, Karen Li, Lilo D. Pozzo
May 2022 Contributed talk	**Materials Research Society Spring Meeting, Honolulu, Hawaii, USA** Autonomous retrosynthesis of nanoscale structures via spectral shape matching **Kiran Vaddi**, Huat Thart Chiang, Lilo D. Pozzo

December 2020 | **Materials Research Society Fall Meeting, Boston, MA, USA**
Contributed talk | High-throughput exploration of materials-phase diagram maps in multi-component organic blends
Kiran Vaddi, Balaji Pokuri, Baskar Ganapathysubramanian, Olga Wodo

October 2020 | **AI for Materials : From Discovery to Production, Webinar,**
Poster | Probabilistic representation of cyclic voltammetry curves for data-driven material discovery
Kiran Vaddi, Olga Wodo

December 2019 | **Materials Research Society Fall Meeting, Boston, MA, USA**
Contributed talk | Accelerating catalyst discovery using Gaussian processes and active learning
Kiran Vaddi, Olga Wodo, Krishna Rajan

May 2019 | **Toyota Research Institute Accelerated Material Design and Discovery Meeting, Boston, MA, USA**
Poster | Machine Learning-Based Simulation Tools for Combinatorial Experiments
Kiran Vaddi, Olga Wodo, Krishna Rajan

Research mentoring

June 2021 – Present | **Graduate student mentoring, Pozzo Research Group, University of Washington, Seattle, WA**
- Kacper Lachowski, Ph.D.
- Huat That Chiang, Ph.D. candidate
- Karen Li, Ph.D. candidate

September 2024 – Present | **Undergraduate student mentoring, Pozzo Research Group, University of Washington, Seattle, WA**
- Aleks Grey, Chemical Engineering.

December 2019 | **Partnerships for Research and Education in Materials (PREM), MRS, 2019, Boston, USA**
- Mentored two undergraduate material science students during their visit to the MRS 2019 Fall meeting.
- Advised mentees towards successful abstract writing, poster competitions, and networking sessions.

Service, Outreach & Leadership

June 2021 – Present | **Academic service**
- **Peer review :** RSC Digital Discovery (**Outstanding Reviewer 2023**), Neural Information Processing Systems (NeurIPS), Journal of Electroanalytical Chemistry, Matter, Nature communications, RSC Advances.
- **Committees :** UW ChemE Distinguished Young Research Scholar Seminar reviewer (2022, 2024), Postdoc representative of 2023 faculty hiring committee.

June 2021 – December 2022 | **Co-chair eScience Postdoc Seminar, University of Washington, Seattle, WA**
- Organized a year-long seminar series for the eScience Institute at the University of Washington, Seattle including invited talks about research and career development.

2020 | **Open source software**
github.com/kiranvad
- **pyMECSim** : Simulating voltammograms of complex multi-step electrochemical reactions in Python.
- **geomstats** : Performing geometric data analysis on functional data.
- **polyphase** : Computing phase diagrams of polymer blends using Flory-Huggins theory.
- **Computational Topology** : Example notebooks introducing topological data analysis.

June 2012 – June 2015 | **National Social Service Scheme, IIT Madras, Chennai, India**
- Awarded **Outstanding Undergraduate Service Award** in 2013 for organizing and mentoring the 'IIT Madras for The Banyan' project.
- Co-organized the inaugural, student-led, interactive support sessions for persons living through poverty and homelessness via The Banyan
- Developed teaching materials and actively participated in community teaching programs.

Professional Memberships

2018 Materials Research Society
2023 Americal Physical Society (DPOLY, DSOFT, GDS)
2023 American Institute of Chemical Engineers (CoMSEF, MESD)
2023 American Chemical Society (COMP, PMSE)