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 Design and Innovation 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

⚙ MACHINE LEARNING

› Reinforcement learning
› Active learning
› Bayesian optimization
› Gaussian processes
› Topological data analysis
› Geometric Statistics

🧪 PHYSICAL SCIENCES

› Material informatics
› Electrochemistry Modelling
› Cyclic voltammetry
› Constitutive modelling
› Thermodynamic phase modelling
› Soft-matter systems

🖧 SOFTWARE SKILLS

› PyTorch, scikit-learn, scipy, pandas
› networkx, scikit-tda, geomstats
› botorch, GPyTorch
› matplotlib, plotly, Bokeh
› Slurm, ray
› LaTeX, C++

🖥 RESEARCH EXPERIENCE

June 2021 Present	**Postdoctoral Research Associate, Department of Chemical Engineering, University of Washington** Advised by Dr. Lilo Pozzo › Developing accelerated material discovery platforms with an emphasis on learning faithful data representations of spectroscopy, scattering characterizations of polymer, colloid and soft-matter systems.
August 2017 June 2021	**Representations for Data-driven Material Discovery** › Developed an automatic metric learning framework for exploratory analysis of combinatorial datasets with comparable accuracy to existing, expert-defined metrics › Developed an oracle based on Gaussian process representation of cyclic voltammetry curves to identifying materials with fast kinetics. (targeted applications in Oxygen reduction and evolution reactions) › Developed a general framework for encoding physics based constraints or prior knowledge into experimental or simulated data by constructing the input data as signals defined on a manifold. Applied this approach to cyclic voltammetry curves for Bayesian optimization framework (in a multi-fidelity environment) to identify optimal mechanism from a set of postulated reaction mechanisms
March 2020 Present	**Thermodynamic phase modelling of polymer solutions** › Developed a framework for high-throughput generation of phase diagrams of polymer solution mixtures using a convex hull minimization of energy landscapes › Applied dimensionality reduction and manifold learning to phase diagrams as a guide to combinatorial design for going beyond the heuristic constructs such as the solubility sphere
March 2020 Present	**Chemical design rules for realizing intermetallics as Quantum materials** › Deriving a structure-property map for electronic properties of Laves phases and Heusler alloys using descriptors based on their elemental constituents › Evaluating the use of classical descriptors governing stability and crystal structure of alloys in design and discovery of intermetallics for modern day applications such as Quantum materials

June 2016 June 2017	**Thermodynamic modelling of photo polymerization** Mentored by Dr.Parag Ravindran at Indian Institute of Technology Madras > Explored construction of constitutive models for diffusion induced deformation of photo polymer under selective irradiation > Theorized a first approximation constitutive model to determine shape of the deformed material as a time varying function of light exposure

✳ AWARDS

June 2021 Present	**UW Data Science Postdoctoral Fellow**, ESCIENCE INSTITUTE, UNIVERSITY OF WASHINGTON, SEATTLE > Awarded to outstanding interdisciplinary researchers who are actively involved in developing and/or utilizing advanced data science tools and techniques in their research at the UW.

🖥 PROJECTS

March 2020 April 2020	**Group Equivariant Q-networks, CSE 510 COURSE PROJECT** > Constructed a group equivariant deep Q-network model to achieve human level control on Atari games in a reinforcement learning environment > Achieved generalizable performance on Atari Pong and Breakout games with minimal re-training for rotated state representations highlighting a equivariant learning from the image pixels
January 2020 February 2020	**Multi-scale topological representations of zeolites, INDEPENDENT PROJECT** > Persistent (co-)homological bar codes are studied as an alternate to graph representation of zeolites to predict inter-zeolite conversion > Successfully classified four types of commonly known inter-zeolite conversion sequences via statistical distribution of distances between vectorized bar codes
November 2017 December 2017	**Data-driven approach to find optimal element for Co-Al alloy formation, MDI 504 COURSE PROJECT** > Developed a framework to identify potential candidates from thirty transition metals for alloy formation in Co-Al using multi-variate statistical approaches such as principal component analysis and spectral clustering > Derived a unsupervised framework and identified key relationships between the electronic and size factors that govern the chemical design rules for alloy formation

🏭 INDUSTRY EXPERIENCE

November 2015 January 2016	**Caterpillar India Pvt.Ltd, Student internship, CHENNAI, TN, India** > Contributed towards a couple of team projects involving thermal analysis of engine gaskets > Developed a framework to perform vibration analysis under a random vibration loading in ABAQUS.
May 2015 July 2015	**Continental Automotive Components India Pvt.Ltd, Student internship, BANGALORE, India** > Developed a theoretical framework of mechanical vibration and failure analysis. > Presented a tutorial on *performing finite element based dynamic analysis of engine components in ANSYS APDL* to a panel of six people

📄 PUBLICATIONS AND PRE-PRINTS

Vaddi, Kiran, Huat Thart Chiang, Lilo D. Pozzo *"Autonomous retrosynthesis of nanoscale structures via spectral shape matching"*
ChemRxiv, 2022, *in peer review*

Lachowski, Kacper J., **Kiran Vaddi**, Nada Y. Naser, François Baneyx, and Lilo D. Pozzo *"Multivariate Analysis of Peptide-Driven Nucleation and Growth of Au Nanoparticles"*
ChemRxiv, 2022, *in peer review*

Vaddi, Kiran, Olga Wodo *"Active knowledge extraction from cyclic voltammetry"*
ChemRxiv, 2021

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.

👥 Conference Proceedings

May 2022 Contributed talk	Materials Research Society Spring Meeting, Honolulu, Hawaii, USA Title : Learning Hierarchical Synthesis Recipes by Spectral Shape Matching and Optimization on Hyperbolic Spaces **Kiran Vaddi**, Huat Thart Chiang, Lilo D. Pozzo
January 2020 Invited talk	IEEE Rochester Section Chapter, Rochester, NY, USA Title : Function Space Data Representation of Temporal Signals for Machine Learning **Kiran Vaddi**
December 2020 Contributed talk	Materials Research Society Fall Meeting, Boston, MA, USA Title : Representations for Data-driven Material Discovery **Kiran Vaddi**,Olga Wodo
December 2020 Contributed talk	Materials Research Society Fall Meeting, Boston, MA, USA Title : High throughput exploration of materials-phase diagram maps in multi-component organic blends **Kiran Vaddi,** Balaji Pokuri, Baskar Ganapathysubramanian, Olga Wodo
October 2020 Poster	AI for Materials : From Discovery to Production, Webinar, Title : Probabilistic Representation of Cyclic Voltammetry Curves for Data-driven Material Discovery **Kiran Vaddi,** Olga Wodo
December 2019 Contributed talk	Materials Research Society Fall Meeting, Boston, MA, USA Title : Accelerating catalyst discovery using Gaussian processes and active learning **Kiran Vaddi,** Olga Wodo, Krishna Rajan
May 2019 Poster	Toyota Research Institute Accelerated Material Design and Discovery Meeting, Boston, MA, USA Title : Machine Learning-Based Simulation tools for Combinatorial Experiments **Kiran Vaddi,** Olga Wodo, Krishna Rajan
December 2018 Poster	Materials Research Society Fall Meeting, Boston, MA, USA Title : Data Analytics for Mapping Catalytic Activity From High Throughput Cyclic Voltammetry **K. Vaddi**, S.V. Devaguptapu, T. Zhang, X. Shen, S. Broderick, E.B. Pitman, F. Yao, O. Wodo, K. Rajan

🖥 Open Source

2020	**Python Electrochemistry Simulation Software**
	🜮 github.com/kiranvad/pyMECSim
	  › A python wrapper for the MECSim software that is capable of simulating voltammograms for complex multi-step reaction mechanisms
	  › pymecsim can be seamlessly integrated to any machine learning framework for example as a multi-fidelity simulator in active or reinforcement learning for catalysis discovery

2019	**Computational Topology**
	🜮 github.com/kiranvad/ComputationalTopology
	  › A collection of iPython notebooks that serves as an introduction to computational topology
	  › Some examples included are identifying cycles and connected components from persistence bar codes, determining circular coordinates for data with one-dimensional loops.

2019	**Weighted Delaunay**
	🜮 github.com/kiranvad/WeightedDelaunay
	  › MATLAB and Python algorithm for finding Delaunay triangulation of point cloud data with scalar weights assigned to each point
	  › Implemented algorithm leverages duality of Delaunay triangulation with convex hull. It can be used for computing Alpha simplices for use in topological data analysis.

⇄ Mentorship, Outreach and Leadership

June 2021	**Co-chair eScience Postdoc Seminar, University of Washington, Seattle, WA** › Responsible for organizing and developing a year long seminar series for the eScience Institute at University of Washington, Seattle.
December 2019	**Partnerships for Research and Education in Materials (PREM), MRS, 2019, Boston, USA** › Mentored two undergraduate material science students during their visit to MRS 2019 Fall meeting. › Advised mentees towards a successful abstract writing, poster competition and networking sessions.
June 2012 June 2015	**National Social Service Scheme, IIT Madras, Chennai, India** › 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.
June 2012 June 2015	Positions of Responsibility Indian Institute of Technology Madras › Student secretary, Ganga Hostel : Elected by an electorate of 400 students to manage and organize socio-cultural events for the academic years 2014-15 › Student coordinator, music events at Saarang : Coordinated a set of three events with over 1000 participants working with a team of ten people.