








Kiran VADDI

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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 Advisors : Dr. Olga Wodo and Dr. Krishna Rajan
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 Advisors : Dr. K.S. Reddy and Dr. Bala Pesala
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

PHYSICAL SCIENCES

- > Material informatics
- > Electrochemistry Modelling
- > Cyclic voltammetry
- > Constitutive modelling
- > Thermodynamic phase modelling

SOFTWARE SKILLS

- > PyTorch, scikit-learn, scipy, pandas
- > networkx, scikit-tda, Ax, GPyTorch
- > matplotlib, plotly, Bokeh
- > Slurm, ray
- > \LaTeX , C++

RESEARCH EXPERIENCE

August 2017 Present	Representations for Data-driven Material Discovery Ph.D Thesis advised by Dr. Olga Wodo and Dr. Krishna Rajan <ul style="list-style-type: none">> 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)> Developing a density based representation of cyclic voltammetry curves for Bayesian optimization framework (in a multi-fidelity environment) to identify optimal mechanism from a set of postulated reaction mechanisms (collaborative project with Dr. Jason Hattrick-Simpers, NIST)
March 2020 Present	Thermodynamic phase modelling of polymer solutions Advised by Dr. Olga Wodo and Dr. Baskar Ganapathysubramanian (Iowa State University) <ul style="list-style-type: none">> 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 Advised by Dr. Krishna Rajan <ul style="list-style-type: none">> 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 <ul style="list-style-type: none">> 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

PROJECTS

March 2020 April 2020	Group Equivariant Q-networks, CSE 510 COURSE PROJECT <ul style="list-style-type: none">> 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 <ul style="list-style-type: none">> 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 <ul style="list-style-type: none">> 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 <ul style="list-style-type: none">> 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 <ul style="list-style-type: none">> Developed a theoretical framework of mechanical vibration and failure analysis.> Presented a tutorial on <i>performing finite element based dynamic analysis of engine components in ANSYS APDL</i> to a panel of six people

PUBLICATIONS AND PRE-PRINTS

Vaddi, Kiran, Olga Wodo, Krishna Rajan. “Active knowledge extraction from cyclic voltammetry”
ACS Analytical Chemistry, *to be submitted*, 2020

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




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
April 2018 Contributed talk	Materials Research Society Spring Meeting, PHEONIX, AZ, USA Title : Metric learning of composition-response mapping from high throughput experiments to accelerate catalyst discovery for fuel cells and metal air batteries K. Vaddi, S. V. Devaguptapu, F. Yao, B. Hayden, K. Rajan, O. Wodo
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

COURSES

Machine Learning	Multivariate statistics and Material Informatics, Experimental Design for Materials Development, Reinforcement Learning
Computational Material Sciences	Electrochemistry, Quantitative Structure Property Relations, Kinetics of Materials and Defects, Numerical Methods in Thermal Engineering
Applied Mathematics	Computational Topology, Visual Group Theory, Introduction to Representation theory
Mechanical Engineering	Mechanics of Viscoelastic Materials, Constitutive Modelling in Continuum Mechanics, Advanced Thermodynamics, Design and Optimization of Energy Systems

OPEN SOURCE

2020	PYTHON ELECTROCHEMISTRY SIMULATION SOFTWARE  github.com/kiranvad/pyMECSim <ul style="list-style-type: none"> > 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 <ul style="list-style-type: none"> > 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 <ul style="list-style-type: none"> > 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

December 2019	Partnerships for Research and Education in Materials (PREM), MRS, 2019, Boston, USA <ul style="list-style-type: none"> > 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 <ul style="list-style-type: none"> > 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 <ul style="list-style-type: none"> > 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.

“ REFERENCES

Krishna Rajan

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