Kiran VADDI

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My main research interests are learning representations for data-efficient scientific discovery and understanding of physical phenomenon. Representations play key role in realizing the dream of autonomous experimental design using techniques such as active learning and reinforcement learning. I am interested in developing frameworks to understand materials based on their topology and (differential) geometry that are both computationally tractable and interpretable.

🏛 EDUCATION

May 2021 August 2017	University at Buffalo, 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

📄 PUBLICATIONS

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

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

👥 CONFERENCES

December 2019	Materials Research Society Fall Meeting, BOSTON, MA, USA Title : Accelerating catalyst discovery using Gaussian processes and active learning **Kiran Vaddi,** Olga Wodo, Krishna Rajan Contributed talk
May 2019	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 Poster Presentation
April 2018	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 Contributed Talk

December 2018	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
	Poster presentation

▤ Skills

Programming	Python, LaTeX
Software Frameworks	PyTorch, scikit-learn, scipy, pandas, Ax, networkx, MATLAB
Visualization	matplotlib, plotly, Bokeh
Computational Material Science	MPRester, pymatgen
Parallel computing	ray
Operating Systems	Mac OS X, Windows, Linux

▦ Industry Experience

November 2015 January 2016	Caterpillar India Pvt.Ltd, Student internship, Chennai, TN, India
	› Understanding dynamical response of engine component systems using finite element analysis
	› 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
	› Developing a theoretical framework of mechanical vibration for prototype vehicle components.

▣ Projects

March 2020 Present	Thermodynamic phase modelling of polymer solutions, Research project, University at Buffalo
	› Using a geometric manifestation of Gibbs stability criterion, determine a phase diagram for polymer-solution mixtures with applications in organic solar cells.
	› Developed a scalable python program to efficiently perform high-throughput phase diagram generation for multi-component polymer mixtures.
	› With Dr. Olga Wodo and Dr. Baskar Ganapathysubramanian
March 2020 Present	Chemical design rules for realizing intermetallics as Quantum materials, Research project, University at Buffalo
	› Deriving a structure-property map for electronic properties of Laves phases and Heusler alloys using descriptors based on their elemental constituents.
	› With Dr. Krishna Rajan at University at Buffalo
March 2020 April 2020	Group Equivariant Q-networks, CSE 510, Spring 2020, University at Buffalo
	› Evaluating the use of a group equivariant deep Q-network model to learn Atari games in a reinforcement learning environment.
	› Achieved generalizable performance with minimal re-training for rotated state representations.
January 2020 February 2020	Topological descriptors to understand zeolite synthesis, Independent project, University at Buffalo
	› Evaluating topological representations of zeolite structures to understand inter-zeolite conversion.
	› Successfully classified four types of commonly known inter-zeolite conversion sequences via their statistical distribution of topological descriptors.
November 2017 December 2017	Data-driven approach to find optimal element for Co-Al alloys, MDI 504, Fall 2017, University at Buffalo
	› Using elemental descriptors, identify design rules for optimal alloy formation for Co-Al alloys.
	› Developed a framework to analyze potential candidate elements using multi-variate statics approaches such as principal component analysis and spectral clustering.

June 2016 June 2017	Thermodynamic modelling of photo polymerization, Independent Research project, IIT Madras › Developing constitutive model for diffusion induced deformation of photo polymer upon selective irradiation with light. › Developing constitutive model to determine shape of the deformed material as a function of incident radiation. › With Dr.Parag Ravindran at Indian Institute of Technology Madras.

📖 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 and TDA, Visual Group Theory
Mechanical Engineering	Mechanics of Viscoelastic Materials, Constitutive Modelling in Continuum Mechanics, Advanced Thermodynamics, Design and Optimization of Energy Systems

💻 Open Source

Pyhton Electrochemistry Simulation Software   2020 - Present
○ github.com/kiranvad/pyMECSim

pymecsim is a python wrapper for the MECSim software that is capable of simulating voltammograms for complex multi-step reaction mechanisms. It can be integrated seemly to any machine learning framework. In my projects, pymecsim was central to the work on GPCV to design experiments for catalyst discovery and cvbayes to identify a mechanism from experimental voltammograms

Python | Electrochemistry | Cyclic voltammetry | Catalysis | Active Learning

Computational Topology   2019 - Present
○ github.com/kiranvad/ComputationalTopology

A collection of iPython notebooks that serves as an introduction to computational topology with emphasis on applications and interpretability.

Topology | Python

Weighted Delaunay   2019 - Present
○ github.com/kiranvad/WeightedDelaunay

A simple program to compute a weighted delaunay of a d-dimensional data. Weighted delaunay can be constructed by using duality with Convex hull of a modified paraboloid and it plays important role in computing Alpha simplices for example.

Topology | Python | MATLAB | Delaunay | Alpha flirtations

⇄ Mentorship, Diversity and Outreach

December 2019	Mentor for Partnerships for Research and Education in Materials (PREM), MRS, 2019, Boston, USA › Mentored two undergraduate material sciences 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-organizer of inaugural student organized interactive support sessions for persons living through poverty and homelessness via The Banyan › Developed teaching materials and actively participated in community teaching programs.

❝ References

Jon Snow	Jon Snow	Jon Snow
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