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 | **University at Buffalo, Buffalo, NY, USA**
August 2017 | PhD in Materials Design and Innovation
Thesis : Representations for data driven material discovery
Advisors : Dr. Olga Wodo and Dr. Krishna Rajan

June 2017 | **Indian Institute of Technology Madras, Chennai, TN, India**
June 2016 | M.Tech in Thermal Engineering
Thesis : Luminescent solar concentrators using high contrast gratings
Advisors : Dr. K.S. Reddy and Dr. Bala Pesala

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

Publications

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.

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**
- 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

Projects

March 2020 – Present | **Thermodynamic phase modelling of polymer solutions, Research project**
With Dr. Olga Wodo Dr. Baskar Ganapathysubramanian
- Evaluating a geometric manifestation of Gibbs stability criteria to determine a phase diagram for polymer-solution mixtures with applications in organic solar cells
- Developing a scalable python program to efficiently perform high-throughput phase diagram generation for multi-component polymer mixtures

March 2020 – Present | **Chemical design rules for realizing intermetallics as Quantum materials, Research project**
With Dr. Krishna Rajan
- 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

March 2020 – April 2020 | **Group Equivariant Q-networks, CSE 510 Course project**
- Evaluated the use of a group equivariant deep Q-network model to learn Atari games in a reinforcement learning environment
- Achieved generalizable performance on Atari Pong and Breakout games with minimal re-training for rotated state representations

January 2020 – February 2020 | **Topological descriptors to understand zeolite synthesis, Independent project**
- Evaluated topological representations of zeolite structures to understand inter-zeolite conversion
- Successfully classified four types of commonly known inter-zeolite conversion sequences via statistical distribution of topological descriptors

November 2017 – December 2017 | **Data-driven approach to find optimal element for Co-Al alloys, MDI 504 Course project**
- Developed a framework to analyze potential candidate elements for alloy formation in Co-Al using multi-variate statistical approaches such as principal component analysis and spectral clustering
- An unsupervised method derived from this project identified key relationships between the electronic and size factors of resulting alloys that govern the chemical design rules for alloy formation

June 2016 – June 2017 | **Thermodynamic modelling of photo polymerization, Independent Research project**
With 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

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
- pymecsim is 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 of catalysis discovery
- 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

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

2019 | **Weighted Delaunay**
github.com/kiranvad/WeightedDelaunay
- Weighted Delaunay implements the algorithm of finding Delaunay triangulation of point cloud data with scalar weights assigned to each point
- Implemented algorithm leverages duality of Delaunay triangulation with Convex hull of a modified paraboloid. The algorithm can be used for computing Alpha simplices for example.

Mentorship, Diversity and Outreach

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.

References

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