# Dilip Krishnamurthy

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## Interests

Deep Learning, Artificial Intelligence, Physics-Informed Machine Learning, Computational Material Design, Electrochemical Systems Modeling, Li-ion Batteries and Fuel Cells, Density Functional Theory (DFT) Simulations

## Education

**Carnegie Mellon University (CMU)** — Pittsburgh, PA
Doctor of Philosophy (Ph.D.) in Mechanical Engineering [GPA: 4.0/4.0] — Fall 2020 (expected)
Advisor: Prof. Venkat Viswanthan

**Indian Institute of Technology Madras (IIT-Madras)** — Chennai, India
Bachelor of Tech. (Hons) and Master of Tech. in Engineering Design [GPA: 9.35/10.0] — June 2015

## Skills

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| **Programming/Tools** | Python, MATLAB, C++, Bash, SQL, LaTeX, Unix, Git |
| **Machine Learning** | TensorFlow, DeepChem, PyTorch |
| **Materials Simulation** | DFT packages (GPAW, VASP), Molecular Dynamics (LAMMPS) |

## Research Experience

**Ph.D. Candidate**, Carnegie Mellon University (Aug 2015 – present) — Pittsburgh, PA

- **Deep Learning to Discover Materials for Electrochemical Ammonia Production**
  - Developed a material-to-performance mapping and identified a novel material that beats the state-of-the-art.
  - Built supervised learning (classification) models trained on experimental data including logistic regression, (kernel) support vector machines (SVMs), decision trees, naive Bayes classifiers and random forest classifiers.
  - Built and optimized the architecture of a deep learning model using TensorFlow to predict KT parameters.
  - Led the closed-loop material design between computation and experiments (Manthiram Group, MIT) and identified 9 novel materials of which 1 material surpasses the Faradaic efficiencies of all reported materials.

- **Prediction of Transition Temperature of Liquid Crystals through a Deep Learning Approach**
  - Curated a dataset of liquid crystals and the associated transition temperatures between various phases.
  - Built an approach to create the input dataset for a classifier given a temperature and a material of interest.
  - Found extended connectivity fingerprints as optimal for classification (crystalline, smectic, nematic, isotropic).
  - Developed and optimized the architecture of a deep learning classifier using TensorFlow to predict the phase of a liquid crystal at a given temperature (accurate within 10° C) based on molecular-scale input features.

- **Engineering the Composition of Solid Electrolyte Interface (SEI) in Li-Metal Batteries**
  - Developed a mechanistic understanding of two high-performing electrolytes (FEC and DFEC) to demonstrate that small structural variations can lead to different decomposition products, and thereby the nature of the SEI.
  - Performed DFT calculations to find two different initial bond-breaking mechanisms between FEC and DFEC.
  - Proposed that the formation of oligomers instead of long polymers may lead to compact SEIs.

- **Computational Design of Cathode Materials for Batteries With Higher Energy Density**
  - Performed atomic-scale (density functional theory) simulations to understand the energetics of several materials to enable rechargeable chemistry and realize the theoretical energy density of lithium-oxygen batteries.
  - Screened through transitional metals for selectivity towards lithium peroxide, the preferred discharge product.
  - Identified 2 noble metals and 1 material from the MXene family of materials that were computed to facilitate rechargeable chemistry with $<$0.2 V overpotential (voltage loss).

- **Machine Learning to Identify Low-Cost (Platinum-Group Metal Free) Materials for Fuel Cells**
  - Developed a neural-network machine learning model to learn the mapping from atomic-scale structure of the catalyst site to the performance. Inverted the machine learning model to identify favorable reaction sites.
  - Identified the nature of active sites where the oxygen reduction reaction occurs on metal sulfide surfaces: 3 sulfur nearest neighbors for Ni-S, similarly for each class of transition metal sulfide.
  - Found that the neural network model and a k-nearest neighbors regression model both perform equally well.
  - Collaborated with experimentalists to successfully test surfaces with higher density of identified optimal sites.
- **Artificial Intelligence and Machine Learning Expertise Through Pet Projects and Courses**
  - Developed a spam classifier by automatically extracting features and using kernel support vector machines.
  - Build a recommender system for movies based on ratings by utilizing collaborative filtering.
  - Implemented a deep convolutional generative adversarial networks (DC-GAN) to generate emojis from samples of random noise. Built a Cycle-GAN to convert between Apple-style and Windows-style emojis.
  - Implemented in OpenAI Gym Markov decision processes (MDPs) for reinforcement learning of agent motion.

**Master's Thesis**, Indian Institute of Technology Madras (Jan 2015 – Aug 2015) Chennai, India

- **Estimation of spatially varying elasto-plastic parameters of structural materials**
  - Performed uniaxial tension tests on specimens sliced out of cylindrical welded stainless steel rods.
  - Imaged specimens during displacement and obtained strain fields through digital image correlation.
  - Computed spatially-varying parameters using the inversion technique of virtual fields method.
  - Correlated the computed parameters with the microstructure of the welded material. Performed principal component analysis (PCA) of the displacement and strain fields to reveal primary deformation patterns.

## Industry Experience

**MRF Tires**, Intern (Jan 2014 – Jan 2015) Chennai, India

- **Mechanical characterization and compositional optimization of tires**
  - Developed a computational method for mechanical characterization (hyperelasticity) of carbon-filled rubbers.
  - Performed experiments to capture 3-Dimensional displacement data using Digital Image Correlation (DIC).
  - Designed and optimized a novel specimen to obtain heterogeneous strains using a planar test setup.
  - The developed model is being used to further optimize the material composition of tires for heavy-duty trucks.

## Select Publications

**D. Krishnamurthy**, N. Lazouski, M.L. Gala, K. Manthiram, V. Viswanathan, "Closed-Loop Design of Hydrogen Donors for Lithium-Mediated Ammonia Production With Interpretable Models and Molecular Machine Learning", Science (in review).

**D. Krishnamurthy**, H. Weiland, A.B. Farimani, E. Anton, J. Green, and V. Viswanathan, "Accelerating Energy Materials Discovery and Optimization through Machine Learning based Approaches", ACS Energy Lett. (2018)

## Book

**D. Krishnamurthy**, B. Ramsundar, V. Viswanathan, "Machine Learning for Physical Systems." (in preparation)

## Select Awards & Honors

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| **Presidential Fellow at Carnegie Mellon University**, the highest fellowship at the university level | 2019–2020 |
| **Bradford & Diane Smith Fellowship**, awarded to a department-nominated Ph.D. candidate | 2018–2019 |
| **Kokes Award**, awarded by the North American Catalysis Society (NACS) | 2017 |
| **Neil & Jo Bushnell Fellowship**, awarded to one department-nominated Ph.D. candidate | 2017–2018 |
| **Sundback Graduate Fellowship**, awarded to one department-nominated Ph.D. candidate | 2016–2017 |
| **Institute Merit Prizes**, the best academic record across the department at IIT Madras | 2014 & 2012 |