

# DILIP KRISHNAMURTHY

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## EDUCATION

### Carnegie Mellon University

Doctor of Philosophy (Ph.D.) in Mechanical Engineering [GPA: 4.0/4.0]

Pittsburgh, PA  
Aug 2015 – May 2021 (expected)

Advisor: Professor Venkatasubramanian Viswanthan

Interests: Computational material design for energy storage and conversion devices; Physics-aware machine learning

### Indian Institute of Technology Madras

B.Tech. and M.Tech. in Mechanical Engineering [GPA: 9.35/10.0]

Chennai, India  
Aug 2010 – Jun 2015

Research advisor: Professor Sankara J. Subramanian

Interests: Inverse design of composite materials through mechanical response characterization using digital image correlation (DIC)

## RESEARCH EXPERIENCE

### Carnegie Mellon University

Ph.D. candidate

Pittsburgh, PA  
Aug 2015 – present

- Implemented machine learning based approaches to predict molecular (solvatochromic) properties of electrolytes for electrochemical ammonia synthesis.
- Developed principles for synergistic design of the electrode-electrolyte assembly for lithium-oxygen batteries.
- Identified the active sites leading to selective electrochemical hydrogen peroxide synthesis using nanowire-templated fuzzy graphene.
- Developed a structure-performance relationship to guide the material synthesis team towards enhanced activity for hydrogen peroxide.
- Developed several approaches for robust prediction of material performance using uncertainty quantification and propagation techniques.
- Mentored multiple students at the undergraduate level and the graduate level.

### National Tsing Hua University

Intern

Hsinchu, Taiwan  
May 2013 – July 2013

- Artificial neural network modeling to devise a novel method in transformer diagnosis to provide a tool for real-time equipment managers. Presented at the International Asia Conference on Industrial Engineering and Management Innovation, National Taiwan University, Taiwan (2013).

## INDUSTRY EXPERIENCE

### MRF Tires

Intern

Chennai, India  
Jan 2014 – Jan 2015

- Developed a robust methodology for material property (hyperelasticity) characterization of carbon-filled rubbers using the eigenfunction virtual fields method.
- Carried out experiments with multiple relaxation steps for obtaining hyperelastic parameters; captured full-field strain data using 3D Digital Image Correlation (3D-DIC). Designed and optimized a novel specimen to obtain heterogeneous strains using a planar test setup.

## PUBLICATIONS

[Google Scholar page](#): Citation Metrics: h-index: 6, i10-index: 3, total citations: 95

*Electrocatalysis for Energy Conversion Devices:*

D.S. Roman<sup>†</sup>, **D. Krishnamurthy**<sup>†</sup>, R. Garg, H. Hafiz, N.T. Nuhfer, V. Viswanathan, and T. Cohen-Karni, "Engineering Three-Dimensional (3D) Out-of-Plane Graphene Edge Sites for Highly-Selective Two-Electron Oxygen Reduction Electrocatalysis." ([arXiv link](#))

**D. Krishnamurthy**, V. Sumaria, and V. Viswanathan, "Quantifying Robustness of DFT Predicted Pathways and Activity Determining Elementary Steps for Electrochemical Reactions." *J. Chem. Phys.* **150**, 041717 (2019)

G. Houchins<sup>†</sup>, **D. Krishnamurthy**<sup>†</sup>, and V. Viswanathan, "The Role of Uncertainty Quantification and Propagation in Accelerating the Discovery of Electrochemical Functional Materials." *MRS Bull.* **44**, 204 (2019)

O. Vinogradova, **D. Krishnamurthy**, V. Pande, and V. Viswanathan, "Quantifying Confidence in Density Functional Theory Predicted Surface Pourbaix Diagrams at Solid-Liquid Interfaces and its Implications for Electrochemical Processes." *Langmuir* **34**, 12259 (2018)

V. Sumaria, **D. Krishnamurthy**, and V. Viswanathan, "Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams and Associated Reaction Pathways for Chlorine Evolution." *ACS Catal.* **8**, 9024 (2018).

**D. Krishnamurthy**<sup>†</sup>, V. Sumaria<sup>†</sup>, and V. Viswanathan, "Maximal predictability approach for identifying the right descriptors for electrocatalytic reactions." *J. Phys. Chem. Lett.* **9**, 588 (2018).

B. Yan<sup>†</sup>, **D. Krishnamurthy**<sup>†</sup>, C. H. Hendon, S. Deshpande, Y. Surendranath, and V. Viswanathan, "Surface Restructuring of Nickel Sulfide Generates Optimally Coordinated Active Sites for Oxygen Reduction Catalysis." *Joule* **1**, 600 (2017).

#### *Material Design for Next-Generation Batteries:*

A. Lee<sup>†</sup>, **D. Krishnamurthy**<sup>†</sup>, and V. Viswanathan, "Exploring MXenes as Cathodes for Non Aqueous Lithium Oxygen Batteries: Design Rules for Selectively Nucleating Li<sub>2</sub>O<sub>2</sub>." *ChemSusChem* **11**, 1911 (2018).

A. Khetan, **D. Krishnamurthy**, and V. Viswanathan. "Towards Synergistic Electrode-Electrolyte Design Principles for Nonaqueous Li-O<sub>2</sub> batteries." *Top. Curr. Chem* **376**, 11 (2018).

**D. Krishnamurthy**, H. A. Hansen, and V. Viswanathan, "Universality in Nonaqueous Alkali Oxygen reduction on Metal Surfaces: Implications for Li-O<sub>2</sub> and Na-O<sub>2</sub> Batteries." *ACS Energy Lett.* **94**, 162 (2016).

#### *Machine Learning Driven Material Design:*

**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.* **4**, 187 (2018)

(equally contributing authors<sup>†</sup>)

#### PATENT

Y-M Chiang, V. Viswanathan, L. Li, V. Pande, **D. Krishnamurthy**, Z. Ahmad, and W. H. Woodford. "Lithium Metal Electrodes and Batteries Thereof." *U.S. Patent 20170288281, WO Patent 2017176936*, October 5, 2017.

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#### SELECT AWARDS & HONORS

<b>Bradford &amp; Diane Smith Fellowship</b> , awarded to a department-nominated Ph.D. candidate	2018
<b>Kokes Award</b> by the North American Catalysis Society (NACS)	2017
<b>Sundback Graduate Fellowship</b> , awarded to one department-nominated Ph.D. candidate	2016
<b>Institute Merit Prizes</b> at IIT Madras for the best academic record in the department	2014 & 2012
<b>Indian Research Internship Program Scholarship</b> , awarded to 23 students in India	2013
<b>Merit Certificate</b> - Indian National Maths Olympiad, awarded to 50 students in India	2010
Rank 16 in the <b>Regional Math Olympiad Karnataka</b>	2010

#### CONFERENCE PRESENTATIONS

**D. Krishnamurthy** and V. Viswanathan, "Robust Activity and Selectivity Predictions in Electrocatalysis from Density Functional Theory Calculations", North American Catalysis Society Meeting, Chicago, IL (2019).

**D. Krishnamurthy** and V. Viswanathan, "Generalized Geometric Descriptors for Oxygen Reduction Activity on Transition Metal Sulfides", American Institute of Chemical Engineers (AIChE) Annual Meeting, Pittsburgh, PA (2018).

**D. Krishnamurthy**, A. Lee, V. Viswanathan, "Exploring the Promise of MXenes as Cathodes for Non-Aqueous Lithium-Oxygen Batteries" (poster), Batteries Conference Gordon Research Conference, Ventura, CA (2018).

**D. Krishnamurthy** and V. Viswanathan, "Geometric Descriptors for the Oxygen Reduction Activity of Transition-Metal Sulfides" (poster), Materials Research Society Fall Meeting & Exhibit, Boston, MA (2017).

**D. Krishnamurthy** and V. Viswanathan, "Structure-Activity Descriptors for Transition Metal Sulfides Reactivity for Oxygen Reduction Reaction", International Society of Electrochemistry Annual Meeting, Providence, RI (2017).

**D. Krishnamurthy** and V. Viswanathan, "Nickel Sulfides as Non-Precious Metal Catalysts for Oxygen Reduction Reaction" (poster), North American Catalysis Society Meeting, Denver, CO (2017).

## TEACHING EXPERIENCE

Spring 2018    **Teaching Assistant**, 24-311 Numerical Methods, Carnegie Mellon University

Spring 2017    **Teaching Assistant**, 24-311 Numerical Methods, Carnegie Mellon University