Dilip Krishnamurthy

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Education

Carnegie Mellon University — Pittsburgh, PA
Doctor of Philosophy (Ph.D.) in Mechanical Engineering [GPA: 4.0/4.0] — May 2020 (expected)
Advisor: Professor Venkatasubramanian Viswanthan
Interests: Interpretable and Physics-Aware Machine Learning; Computational Material Design for Energy Storage and Conversion Devices.

Indian Institute of Technology Madras — Chennai, India
Bachelor of Technology and Master of Technology in Mechanical Engineering [GPA: 9.35/10.0] — June 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 (Aug 2015 – present) — Pittsburgh, PA

- Implemented a data-driven approach based on deep learning to identify novel proton sources that enable electrochemical ammonia synthesis, a cutting-edge alternative to the emissions-intensive Haber-Bosch process.
  - Performed rigorous model selection for robust predictions in the "small-data" regime of machine learning.
  - Developed a framework involving molecular featurization (from SMILES IDs) of proton sources followed by a multi-task neural network to predict solvatochromatic parameters, fed into a trained Leisen-Reimer regression tree to predict ammonia yields.
  - Partnered with my experimental collaborators and identified at least 3 new tested proton sources that surpass the yields of the few known modest proton sources.
- Identified through the inversion of machine learning models (trained on atomic-scale simulation results) the precise nature of active sites where the oxygen reduction reaction occurs on transition metal sulfide materials.
  - Developed a relationship between the atomic-scale structure of the catalyst site and the performance, for which a neural network model and a k-nearest neighbors regression model both perform equally well.
  - Inverted the relationship to identify the optimal nature (3 sulfur nearest neighbors for Ni-S) of active sites.
  - Partnered with experimental collaborators to successfully test the identify optimal catalytic sites. Guiding experimental collaborators to synthesize and test other promising transition metal sulfides.
- Identified promising cathode materials that can circumvent inherent rechargeability issues associated with lithium-oxygen batteries.
  - Designed the electrochemistry to enable selectivity towards rechargeable products at the cathode.
  - Performed density functional theory (DFT) calculations to assess various noble metals that can be used for oxygen reduction with lithium ions.
- Mentored multiple (6 total) students at the undergraduate level and the graduate level.

Skills

Programming Languages	Proficient: Python, MATLAB Knowledgeable: Bash, C, C++, SQL, Java
Deep Learning Frameworks	TensorFlow, DeepChem, PyTorch
Materials Simulation	DFT packages (GPAW, VASP), Molecular Dynamics (LAMMPS)
Tools	LaTeX, Unix, Git

Publications

Google Scholar page: Citation Metrics: h-index: 7, i10-index: 5, total citations: 129

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)

Material Design for Next-Generation Batteries:

A. Lee†, **D. Krishnamurthy**†, and V. Viswanathan, "Exploring MXenes as Cathodes for Non Aqueous Lithium Oxygen Batteries: Design Rules for Selectively Nucleating Li_2O_2." ChemSusChem 11, 1911 (2018).

A. Khetan, **D. Krishnamurthy**, and V. Viswanathan. "Towards Synergistic Electrode-Electrolyte Design Principles for Nonaqueous Li-O_2 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_2 and Na-O_2 Batteries." ACS Energy Lett. 94, 162 (2016).

Electrocatalysis for Energy Conversion Devices:

D.S. Roman†, **D. Krishnamurthy**†, 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." ACS Catal. (2020)

Y. Kim, S. Xu, J. Park, A. Lal Dadlani, O. Vinogradova, **D. Krishnamurthy**, M. Orazov, D. Lee, S. Dull, H. Han, Z. Wang, T. Graf, T. D. Schladt, J. E. Mueller, R. Sarangi, R. Davis, V. Viswanathan, D. Higgins, T. F. Jaramillo, F. Prinz, "Atomic Layer Deposition Prepared Platinum-Titanium Alloys for Oxygen Reduction Reaction" (submitted)

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

B. Yan†, **D. Krishnamurthy**†, 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). **Highlight Article Link**

(equally contributing authors†)

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. **Licensed by 24M Technologies Inc.**

Select Awards & Honors

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 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 at IIT Madras for the best academic record in the department 2014 & 2012
Indian Research Internship Program Scholarship, awarded to 23 students in India 2013
Merit Certificate - Indian National Maths Olympiad, awarded to 50 students in India 2010