

Artificial Intelligence Strategies for Materials Discovery with Explainable and OpenSharing Capabilities



Prof. Prasanna V. Balachandran

Materials Informatics Group

Department of Materials Science and Engineering & Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville

Date & Time- September 30th, 2022 at 10 AM ET

SEMINAR LINK- <https://www.youtube.com/channel/UCAwzWog7PqFw5R0q90KI6KQ/featured>

Abstract:

In this talk, I will discuss some of the past and on-going research in the application of machine learning methods to efficiently guide materials design and discovery efforts. The overarching theme is in the efficient navigation of the vast search space, which is especially critical when brute-force evaluation of the search space is prohibitively expensive. Adaptive learning methods, such as active learning and Bayesian optimization, provide a promising solution to address this important problem. One of the expected outcomes from an iterative adaptive learning loop is an improved black-box machine learning or surrogate model that is believed to capture the complexity of the structure-property relationships with sufficient accuracy. More recently, our group has expanded the adaptive learning paradigm in two directions: (1) Incorporating novel post-hoc model explainable methods to peek inside the trained black-box models and explain the predictions for each observation in the data set. (2) Build Web Applications that will allow the public to interact with our trained models and accelerate discoveries.

Bio:

Prof. Prasanna Balachandran is currently an Assistant Professor in the Department of Materials Science and Engineering with a joint appointment in the Department of Mechanical and Aerospace Engineering at the University of Virginia (UVA). He earned his Bachelors' Degree in Metallurgical Engineering from Anna University, India in 2007 and Ph.D. in Materials Science and Engineering from Iowa State University, USA in 2011. Prior to joining UVA in December 2017, he spent three and half years as a postdoctoral research associate in the Theoretical Division at Los Alamos National Laboratory (LANL), USA and two years as a postdoctoral research associate at Drexel University, USA. His research interests are in the application of first-principles based density functional theory calculations and information science methods for accelerating the design and discovery of new materials.