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Thursday, January 16, 2020, 9:15-10:15 am

Armstrong Hall of Engineering, Room B071

Data-Driven Design of Energy Materials



Dr. Arun Kumar Mannodi Kanakkithodi is a postdoctoral researcher at Argonne National Laboratory working in the Theory and Modeling group at the Center for Nanoscale Materials. He received his bachelors degree in Metallurgical and Materials Engineering from Indian Institute of Technology Roorkee in 2012 and his PhD in Materials Science and Engineering from the University of Connecticut in June 2017. His research focuses on first principles-based materials simulations and machine learning-driven design and discovery of new materials for energy relevant applications. During his PhD, he used high-throughput computation and machine learning to drive the experimental discovery of novel polymers for capacitor dielectrics, as well as the creation of an online informatics platform for polymer discovery, The Polymer Genome (<https://www.polymergenome.org/>). At Argonne, Arun works in close collaboration with experimental colleagues and computer scientists to accelerate the prediction of structural, electronic, optical and defect properties of semiconductors belonging to various classes such as halide perovskites and chalcogenides, for application in the areas of photovoltaics and optoelectronics.

Abstract: Growing technological and energy needs have made the efficient design of novel materials ever more imperative. This has resulted in fascinating innovations that center around the use of first-principles computations on a large scale by exploiting advances in theory and high performance computing, the application of machine learning or artificial intelligence to diverse materials data, and the implementation of a rational co-design strategy wherein experiments and computations performed in a synergistic manner drive continuous discovery and insights. In this talk, I will present examples from my research that combine all these different aspects leading to the development of general materials design frameworks for energy applications such as solar cells and capacitors. Models are trained for prediction of properties in an "on-demand" fashion, high-throughput screening is performed based on computed or machine-learned properties, and targeted experiments carried out by collaborators result in validation and discovery. Through my talk, I hope to illustrate how computational data and machine learning are leading to definitive, transferable, reproducible and generalizable data-driven solutions for materials design, setting the materials science community well on its way to achieving the goals of the Materials Genome and AI initiatives.