ME Seminar

Functional Materials by Design – High Throughput Experiments and Computations with Machine Learning

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ABSTRACT

The design of electronic and thermal materials, both purely inorganic compounds as well as inorganic-organic hybrids is a difficult challenge due to the large state space in the Structure-Process-Property-Performance paradigm. The process of Materials-by-Design constitutes multiple steps including (A) invertible representations of structure, followed by (B) creation of a database of out-of-equilibrium functional properties, and finally (C) Machine Learning models. Synthesis of new materials and composites requires process parameter tuning, where Bayesian Optimization is powerful. I will describe our efforts to design new inorganic thermoelectric materials, predicting their performance via machine learning models, and end with the description of a High-Throughput Experimental platform that can synthesize and rapidly characterize new materials in thin film form with high electrical conductivity. The ability to generate new materials with desired properties is possible through the development of materials descriptors; I will describe our efforts at using High-Performance Computing to produce such new electronic descriptors for thermoelectrics.

ABOUT THE SPEAKER

Asst. Prof. Kedar Hippalgaonkar is a joint appointee with the Materials Science and Engineering Department at Nanyang Technological University (NTU) and as a Senior Scientist at the Institute of Materials Research and Engineering (IMRE) at the Agency for Science Technology and Research (A*STAR). He did his PhD in Mechanical Engineering from Prof. Arun Majumdar's group in UC Berkeley studying phonon physics at the nanoscale. After moving to Singapore in 2014, he started and led a $12M research Program on hybrid (inorganic-organic) thermoelectrics 2016-2020. Currently, he is leading the Accelerated Materials Development for Manufacturing (AMDM) program from 2018-2023 focusing on the development of new materials, processes and optimization using Machine Learning, AI and high-throughput computations and experiments. Dr. Hippalgaonkar's interests are in designing functional materials, especially for energy applications building upon principles in solid state physics, 1D (nanowires), 2D (TMDCs) as well as inorganic-organic (hybrid) materials.

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