NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

School of Materials Science and Engineering

Seminar Topic:
Materials by Design – High Throughput Experiments, Simulations and Machine Learning

Assistant Professor Kedar Hippalgaonkar

Abstract

Designing and synthesizing materials with desired functional properties is a key challenge. With the recent advances in machine learning, the ability to perform automated experiments and high-performance simulations, new tools have emerged that allow for the acceleration of the materials discovery process. In this talk, first I will discuss how we have used machine learning models to not only predict good thermoelectric materials from existing databases (e.g. Materials Project), but also tune the machine learning models to predict previously unseen new compounds. Following this, I will talk about our results on the generation of materials databases, both computationally and experimentally. With a focus on electronic materials, Density Functional Theory, followed by high-throughput charge scattering time calculations allow us to calculate the electron mobility, Seebeck coefficient and electrical conductivity of a large number of inorganic compounds. This is a high fidelity database that can be utilized by machine learning in the future. In terms of high-throughput experiments, I will share our progress on the flow-based synthesis, dropcast thin film formation and optical/electrical characterization tool, which allows for collection of labeled datapoints for inorganic-organic hybrid materials – here we navigate a complex parameter space by using Bayesian optimization.

Biography

Prof. Kedar Hippalgaonkar is a joint appointee with the School of Materials Science and Engineering 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 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 in electronic and plasmonic materials and polymers. He is also leading the Pharos Program on Hybrid (inorganic-organic) thermoelectrics for ambient applications from 2016-2020.

He has published over 50 research papers, and was nominated as a Journal of Materials Chemistry Emerging Investigator in 2019. He was recognized as a Science and Technology for Society Young Leader in Kyoto in 2015. For his outstanding graduate research, he was awarded the Materials Research Society Silver Medal in 2014. He graduated with a Bachelor of Science (Distinction) from the Department of Mechanical Engineering at Purdue University in 2003 and obtained his Doctor of Philosophy from the Department of Mechanical Engineering at UC Berkeley in 2014. While pursuing his doctoral studies, he conducted research on fundamentals of heat, charge and light in solid state materials.

Wednesday, 12 February 2020 ǁ Time: 2:00 pm – 3:00 pm ǁ
Venue: MSE Meeting Room (N4.1-01-28)
Hosted by: Associate Professor Andrew C. Grimsdale

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