IMS Seminar

Friday, February 21, 2025
11:45 AM, Science 1 - Room G01

**Snacks, coffee, and tea will be served beginning at 11:30 a.m.*

CELEBRATING OUR 60TH ANNIVERSARY
1965 - 2025
IMS INSTITUTE OF MATERIALS SCIENCE

Dr. Arun Mannodi Kanakkithodi
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Purdue University
Ph.D. Materials Science and Engineering ('17)
UConn Materials Science & Engineering Department
(Advisor: Dr. Rampi Ramprasad (Former UConn MSE Professor))

Rational Computational Design of Next-Generation Semiconductors

Abstract: Challenges of environmental pollution, global energy shortage, and overreliance on fossil fuels can be addressed by innovation in solar technology, such as new absorbers for increasing solar cell efficiency and improved photocatalysts for hydrogen production and CO2 reduction. Novel semiconductors that show bulk stability, promising optical and electronic properties, defect tolerance, and suitable dopability, are desired as substitutes for current candidates used in these applications. However, the atom-composition-structure space of potential materials is practically infinite and not conducive to brute-force experimentation or computation. This necessitates the use of data-driven strategies combining large computational datasets and state-of-the-art machine learning (ML), prior to experimental validation and discovery. Provided a sufficiently diverse dataset of accurate property estimates can be generated from density functional theory (DFT), and materials can be suitably encoded using chemical "descriptors", DFT-ML models can be trained to enable millions of new predictions at expensive DFT accuracy but a mere fraction of the cost. Such DFT-ML models can be trained synergistically within a multi-fidelity framework by combining data from different functionals with collaborative experiments, ultimately leading to high-fidelity selection of the "needle in the haystack", i.e., the best candidates out of infinitely many. In this talk, I will discuss how we apply these ideas in the Mannodi research group to drive the discovery of novel semiconductors for solar absorption and photocatalysis. By combining high-throughput DFT, multi-fidelity active learning, and crystal graph-based neural networks, we successfully designed dozens of novel halide and chalcogenide compounds with suitable thermodynamic stability, electronic band gaps and edges, optical absorption behavior, intrinsic defect tolerance, and ability to be doped. I will further discuss work done in my group to advance open-science and education via DFT datasets and ML tools created as part of nanoHUB, a nanotechnology repository housed at Purdue.

Biography: Arun Mannodi Kanakkithodi is an assistant professor in the department of Materials Engineering at Purdue University. He spent 5 memorable years at UConn, receiving his PhD in Materials Science and Engineering in 2017, working in Prof. Rampi Ramprasad's group. Arun worked as a postdoctoral researcher at Argonne National Laboratory from 2017 till 2020. His research primarily involves applying first principles simulations and methods rooted in data science and machine learning for materials design. He is a contributor to and co-organizer of machine learning resources and hands-on workshops for nanoHUB, and a regular organizer of materials informatics tutorials at Materials Research Society (MRS) fall and spring meetings. Arun is a recipient of the 2020 Distinguished Young Investigator award from Argonne, the 2023 Functional Materials Division (FMD) Young Leaders Professional Development Award from TMS, a 2023 DOE Solar Energy Technology Office (SETO) Small Innovation Projects in Solar (SIPS) awardee, and a 2024 ACS Materials Au Rising Star in Materials Science.

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