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Towards AI-Driven Discovery of Renewable Energy Materials: Thermoelectrics, Semiconductors, Catalysts, and More

The increasing availability of data from the first three paradigms of science (experiments, theory, and simulations), along with advances in artificial intelligence and machine learning (AI/ML) techniques has offered unprecedented opportunities for data-driven science and discovery, which is the fourth paradigm of science. Within the arena of AI/ML, deep learning (DL) has emerged as a game-changing technique over the last decade with its ability to effectively work on raw big data, bypassing the (otherwise crucial) manual feature engineering step traditionally required for building accurate ML models, thus enabling numerous real-world applications, such as autonomous driving. In this talk, I will present our ongoing research in interdisciplinary AI, along with its real-world applications in science and engineering. In particular, we will see how AI/ML/DL can be used to learn the forward and inverse processing structure-property-performance (PSPP) relationships in various materials systems, including for renewable energy materials, such as thermoelectrics and semiconductors, as well as to accelerate nanocombinatorics workflows to facilitate rapid structure characterization and discovery of catalysts. I will also demonstrate some of the software tools deploying AI for materials developed in our group.

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Biography

Dr. Ankit Agrawal (Ph.D. 2009, B.Tech. 2006) specializes in interdisciplinary AI and is a pioneer in materials informatics (AI for materials). He has co-authored 200+ publications with 15,000+ citations (h-index: 50+), co-developed 20+ software, delivered 75+ invited/keynote talks, and served as a PI/Co-PI on 20+ projects with a combined budget of over \$100 million, funded by US federal agencies (e.g., NSF, DOE, AFOSR, NIST) as well as industry (Toyota Motor Corporation Japan). He has been featured in Stanford/Elsevier's list of top 2% scientists, as well as named a ScholarGPS Top Scholar for being in top 0.5% of scholars worldwide.