Machine Learning Accelerates the Diagnosis, Process Optimization, and Discovery of Novel Energy Materials

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Reception 3:30-4:00 p.m. | NANOENGINEERING 181

Lecture 4:00-5:00 p.m. | NANOENGINEERING 181

Abstract

We envision a scientific laboratory where the process of materials discovery continues without disruptions, aided by computational power augmenting the human mind, and freeing the latter to perform research closer to the speed of imagination, addressing societal challenges in market-relevant timeframes. — "Accelerating Materials Development via Automation, Machine Learning, and High-Performance Computing," *Joule* **2**, 1410 (2018)

In this talk, I'll describe how machine learning (ML) is ripe to disrupt three R&D tasks: **diagnosis**, **process optimization**, and **discovery**. "Diagnosis" in this context refers to the purposeful application of characterization to identify underlying performance-limiting physics, an essential step toward improving early-stage prototypes. ML can increase diagnosis speed and efficiency. As examples, I'll demonstrate how Bayesian inference accelerates 10x root-cause diagnosis of under-performing early-stage photovoltaic devices, and convolutional neural networks enable rapid and interpretable classification of X-ray diffraction spectra. Accurate diagnosis directs "process optimization," which can help determine the performance ceiling of novel materials, and when to abandon unsuccessful candidates quickly. Lastly, materials screening, in combination with high-throughput experimentation enabled by ML, can lead to novel materials "discovery," as we illustrate with the case of novel lead-free perovskite-inspired photovoltaic materials with promising optoelectronic properties, and poly(2-oxazoline) block co-polymers with user-customized cloud-

point transition temperatures. In conclusion, I'll illustrate how these principles generalize to other systems, and promise to accelerate the cycle of learning by ≥10x across a range of chemistry and materials disciplines.

Bio

Tonio Buonassisi is a Professor of Mechanical Engineering at the Massachusetts Institute of Technology (MIT). He is pioneering the application of artificial intelligence to develop new materials for societally beneficial applications. His research in solar photovoltaics and technoeconomic analysis assisted technology developments in dozens of companies, earning him a US Presidential Early Career Award for Scientists and Engineers (PECASE), a National Science Foundation CAREER Award, and a Google Faculty Award. He founded the MIT PVLab and co-founded the Fraunhofer Center for Sustainable Energy Systems in Boston USA. A recipient of the prestigious MIT Everett Moore Baker Memorial Award for Excellence in Undergraduate Teaching, his passion for education is evidenced by the >73k views of his OpenCourseware/YouTube PV lectures series, and a recent AI-focused YouTube video series "Accelerated Materials Development for Manufacturing."