AI-Driven Autonomous Sustainable Materials Engineering Platforms

Dr. Filippos Tourlomousis, PhD

Founder & Chief Scientist @ Superlabs (www.superlabs.eu)
Founder & CEO @ Biological Lattice Industries, Corp. (www.biolattice.ai)
Research Associate @ National Center of Scientific Research Demokritos, Greece

Abstract:
There is a growing interest to leverage data-driven models (AI and ML) to help discover new materials, accelerate material optimization, and lower costs by reducing expensive laboratory measurements. However, building data-driven models and eliminating experiments are often mutually exclusive ideas in scientific discovery. The strength of data-driven models is directly proportional to the amount and quality of data that they are trained on, and experiments are where these data are produced. Thus, this vision of simulation and AI-driven exploration and design relies on a significant change to the status quo in many laboratories. In this lecture, I will describe how AI-driven exploration and design will shape the sustainable materials labs of the future for accelerating the discovery and optimization of new materials for the circular economy. With experimental data disseminated on open-source materials databases, statistical and machine learning models can be built where users specify material performance targets, and the model generates specific formulation and process parameters that meet these targets. Such models can be useful to potential local and regional producers, enabling the material production process to be tailored to customer needs. However, the search for novel and improved functional sustainable materials necessitates the exploration of increasingly complex multi-component materials. With each new component or materials parameter, the space of candidate experiments grows exponentially. High-throughput synthesis and characterization techniques offer a partial solution: with each newly added composition parameter, the number of candidate experiments becomes intractable, and thus exhaustive exploration becomes infeasible. The search is further confounded by the chemical heterogeneity and the complex Processing-Structure-Property-Performance landscape of materials relationships. Coupled with the sparsity of optimal materials, these challenges threaten to impede innovation and industrial advancement. Proper machine learning tools coupled with autonomous materials engineering systems could help innovators and scientists to fail smarter, learn faster, and spend less on experimental resources, while simultaneously strengthening the reproducibility of their generated materials data. In this lecture, we will outline with specific examples how the future of sustainable materials discovery and adoption will be defined by the effective collaboration of material scientists with robots and computers by increasing data throughput and importantly lowering the cost per data point.