TMS | ONLINE COURSE

# ARTIFICIAL INTELLIGENCE IN MATERIALS SCIENCE AND ENGINEERING


**November 2–4, 2021** • This course will include five, half-day, virtual modules, with supporting materials.

*Instructional sessions will be recorded and available to participants for a limited time after the course concludes.*

## COURSE MODULES

**Module 1: The Road to AI: A Historical and Computational Perspective**
This module will review the evolution of AI from a historical perspective. It will then provide a high-level overview of some key components of AI that will be covered in much more detail in the subsequent modules. Here, the focus will be specifically on components that are employed in materials science and engineering, and materials-related manufacturing, including machine learning (and deep learning), computer vision, natural language processing, and autonomous research. Finally, some specific case studies of the application of AI in materials research and design will be provided.

**Module 2: Introduction to Machine Learning and Deep Learning for Materials Science**
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 in recent years 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. This module will introduce some of the fundamental concepts in AI/ML/DL along with illustrative examples of their application in materials science and engineering. We will discuss the unique aspects of applying AI/ML/DL to materials science specifically, and also how to be an informed "consumer" of these data-driven models.

**Module 3: Computer Vision for Microstructural Analysis**
Computer vision incorporates AI tools such as convolutional neural networks (CNNs) and machine learning to extract information from images. When applied to materials science images, computer vision enables autonomous and high-throughput analysis, including classification, segmentation, and characterization. In this module, we will introduce computer vision for microstructural image analysis through lectures and a hands-on tutorial.

**Module 4: Autonomous Research: Theory and Implementation**
This tutorial describes the basic theory underpinning many autonomous closed-loop research platforms. Additionally, we describe the practical process of connecting the developed models and algorithms to machine-controllable equipment. Finally, we close with a discussion of various software tools relevant to autonomous research.

**Module 5: AI/ML for Materials Manufacturing: Understanding the Applications, Building Predictive Modeling, and Uncertainty Quantification**
The first half of this module will review production examples of applications of data collection and machine learning in production manufacturing environments. With a focus on aluminum die casting, topics including data collection misclassifications, dealing with highly unbalanced data sets, data space overlap, and cost/accuracy needs of machine learning (ML) systems will be reviewed. In the second half, we will discuss probabilistic machine learning focusing on building Gaussian Process model and demonstrate its use for predictive modeling, uncertainty quantification, and sensitivity analysis. Lastly, we will discuss active learning or intelligent experimentation, which can reduce experimental cost for model building by ML-enhanced intelligent decision making for experimental planning. Jupyter notebook (with Python) will be used to demonstrate the modeling process vis simple examples. Hand-on activity: attendees will apply Prob-ML code using their formatted dataset and model results will be briefly discussed at the end of the workshop.

**Learn more about the curriculum and the team of 10 expert instructors and register:**
**www.tms.org/AIcourse**