

# PREDICTIVE MULTISCALE MATERIALS DESIGN

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PROFESSIONAL EDUCATION 

## OVERVIEW

Computational methods including AI is revolutionizing the materials design world. Today, an engineer or scientist can simply enter the desired properties into a program and the system will manufacture a microstructure that matches the specifications. Algorithms predict which chemical building blocks can be combined to create advanced materials with superior functions—from ultra-strong, lightweight materials used in the automotive, construction and aerospace industries, to biomaterials used in implants and biomedical devices with the ability to self heal and regenerate.

This course covers the science, technology, and state-of-the-art computing methods being used to fabricate innovative materials from the molecular scale upwards, as well as advanced manufacturing methods, such as additive manufacturing. Through lectures and hands-on labs, participants will learn how to construct, in a bottom-up manner, atomically-precise products through the use of molecular design, predictive modeling, and manufacturing, allowing the fabrication of a vast array of advanced, innovative designs for a wide-range of applications. You'll explore:

- Cutting-edge computational tools that range from multi-scale modeling to the use of machine learning and AI
- How to use the tools to predict mechanical properties such as strength, toughness, deformability, and elasticity, as well as optical, thermal, and electronic properties
- How superior material properties in nature and biology can be mimicked in bio-inspired materials
- The synthesis of computationally-designed hierarchical composites using 3D printing and other advanced manufacturing techniques, followed by subsequent mechanical testing

This course was previously titled *Multiscale Materials Design*.

## EARN A PROFESSIONAL CERTIFICATE IN MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE

This course may be taken individually or as a part of the Professional Certificate Program in Innovation & Technology or the Professional Certificate Program in Design & Manufacturing. Learn more at [shortprograms.mit.edu/mlai](https://shortprograms.mit.edu/mlai).

## LEAD INSTRUCTOR:

Markus J. Buehler

**COURSE DATES:** June 1 - 5, 2020

**COURSE LENGTH:** 5 days

**COURSE FEE:** \$4,500

**CEUs:** 2.9

## WHO SHOULD ATTEND

This course will be of interest to scientists, engineers, managers, and policy makers working in the areas of materials design, development, manufacturing, or testing, who are interested in understanding how to optimize a material's structure and performance. It should appeal to anyone working in materials or in an industry that builds on a material interaction platform (such as pharmaceuticals, regenerative medicine, energy, or other engineering materials such as concrete) and who is interested in understanding how to optimize a material's structure and performance. The focus on mechanical properties will include domains such as biomaterials and implants, adhesives, construction materials, and structural materials for the aero-astro, manufacturing, and automotive industries. There are no prerequisites for the course.

**Computer Requirements:** Laptops are required for this course. Software used will include Visual Molecular Dynamics and web-based tools. Tablets will not be sufficient for the computing activities performed in this course.

**REGISTER** and learn more at [shortprograms.mit.edu/mmd](https://shortprograms.mit.edu/mmd) or email [shortprograms@mit.edu](mailto:shortprograms@mit.edu)

# PREDICTIVE MULTISCALE MATERIALS DESIGN

## PARTICIPANT TAKEAWAYS

- Practical problem-solving computational tools paired with a detailed discussion of experimental techniques to probe, understand, and design the ultimate structure of materials—from atoms upwards
- How to use the tools to predict mechanical properties such as strength, toughness, deformability, and elasticity, as well as optical, thermal, and electronic properties
- How to use multiscale tools in energy recovery and sustainable materials and structures
- Demonstrate the synthesis of computationally-designed hierarchical composites using 3D printing and other advanced manufacturing techniques, followed by subsequent mechanical testing. Includes validation of computational predictions, focused on fracture toughness and strength
- Critically evaluate and apply the use of computational tools in materials design (synthesis and testing)—molecular mechanics, nanotechnology, multiscale and hierarchical materials, and emerging materials technologies
- The fundamentals and codes to perform state-of-the-art techniques, such as molecular dynamics, molecular mechanics, and coarse-graining, used to cover a range of length- and time-scales



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## INSTRUCTOR



**MARKUS J. BUEHLER** is the McAfee Professor of Engineering at MIT and directs the Laboratory for Atomistic and Molecular Mechanics (LAMM). A world-renowned researcher and engineer, he is the Principal Investigator on numerous national and international research programs. Buehler's primary research interest is to identify and apply innovative approaches to design better materials from less, using a combination of high-performance computing, new manufacturing techniques, and advanced experimental testing. He combines bio-inspired materials design with high-throughput approaches to create materials with architectural features from the nano- to the macro-scale, and applies them to various domains that include composites for vehicles, coatings for energy technologies, and innovative and sustainable construction materials.

Buehler is a sought-after lecturer and has given hundreds of invited, keynote, and plenary talks throughout the world. His scholarly work is highly-cited and includes more than 450 articles on computational materials science, biomaterials, and nanotechnology, many in high-impact journals such as *Nature*, and *Proceedings of the National Academy of Sciences*. He authored two monographs in the areas of computational materials science and bio-inspired materials design, and is a founder of the emerging research area of materiomics. He is a dedicated educator and a gifted teacher, and has appeared on numerous TV and radio shows to explain the impact of his research to broad audiences. In 2016 Prof. Buehler was awarded the Foresight Institute Feynman Prize for his advances in nanotechnology, and was chosen as the 2018 Materials Horizons Prize recipient, among many other awards and recognitions. He is a Clarivate Highly Cited Scientist.

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