

MULTISCALE MATERIALS DESIGN

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JUNE 12-16 2017
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Learn how to design and manufacture better materials from less

As the demand for high-performance materials with superior properties, flexibility, and resilience grows, a new design paradigm from the molecular scale upwards has revolutionized our ability to create novel materials. This course covers the science, technology, and state-of-the-art in atomistic, molecular, and multiscale modeling, synthesis and characterization. Through lectures and hands-on labs, participants will learn how superior material properties in nature and biology can be mimicked in bioinspired materials for applications in new technology. The course also covers sustainable infrastructure materials such as concrete and asphalt and technologies for energy extraction. Bridging multiple hierarchies of length- and time-scales, this course trains participants in applications to polymers, composites and metals.

The course will focus on practical problem-solving computational tools paired with a detailed discussion of experimental techniques to probe the ultimate structure of materials, emphasizing tools to predict key mechanical properties. Case studies of molecular mechanics, bio-inspired composites, and dynamic fracture of composites and polymers will be presented and carried out by participants in computational labs. Simulation codes, algorithms, and details of the implementations of different simulation technologies, including validation, will be presented, including practical issues such as supercomputing (hardware and software), parallelization, Graphics Processing Computing (GPU), and others. A specific

focus is on structural polymers and composites, including innovative material platforms such as carbon nanotubes, graphene, and protein materials.

What you will learn

- 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
- Learn how to use the tools to predict mechanical properties such as strength, toughness, deformability, and elasticity, as well as optical, thermal and electronic properties
- Learn how to use multiscale tools in energy recovery and sustainable materials & structures, including biomaterials
- Demonstrate the synthesis of computationally designed hierarchical composites using 3-D printing and other advanced manufacturing techniques, followed by subsequent mechanical testing. Includes validation of computational predictions, focused on fracture toughness and strength and other value-added material properties
- Critically evaluate & apply the use of computational tools in materials design (synthesis & testing) – molecular mechanics, nanotechnology, multiscale/hierarchical materials, and emerging technologies
- Participants will learn 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.
- A new paradigm to make revolutionary advances in conventional technologies, by introducing a bottom-up design paradigm, to create innovative material solutions for use in a variety of fields, including infrastructure and environment

Who should enroll

Scientists, engineers, or employers from any industry in materials or that builds on material interaction platforms (mechanical and civil, defense and other industries, pharmaceuticals, regenerative medicine, energy and construction materials) who are interested in understanding how to optimize a material's structure and performance. There are no prerequisites for this course and it is accessible for a diverse audience.

About the instructor

Markus J. Buehler is the McAfee Professor of Engineering at the Massachusetts Institute of Technology and Head of the MIT Department of Civil and Environmental Engineering. He is an internationally renowned materials scientist and directs MIT's Laboratory for Atomistic and Molecular Mechanics (LAMM), leads the MIT-Germany program, and is 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 range from composites for vehicles, biomaterials, biomedical applications, coatings for energy technologies, to innovative and sustainable construction materials.



Professor 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 300 articles on computational materials science, biomaterials and nanotechnology, many in high-impact journals such as Nature, Science Advances, and PNAS. 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 has appeared on many TV and radio shows to explain the impact of his research to broad audiences. Buehler received the TMS Hardy Award, the MRS Outstanding Young Investigator Award, the ASME Thomas J. R. Hughes Young Investigator Award, the ASME Sia Nemat-Nasser Medal, the ASCE Rossiter W. Raymond Memorial Award, the ACS Stephen Brunauer Award, the ASCE Alfred Noble Prize, and the Leonardo da Vinci Award given by the Engineering Mechanics Institute of ASCE. He is a recipient of the National Science Foundation CAREER award, the United States Air Force Young Investigator Award, the Navy Young Investigator Award, and the Defense Advanced Research Projects Agency (DARPA) Young Faculty Award, as well as the Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the United States government on outstanding scientists and engineers in the early stages of their careers. He was an invitee at several National Academy of Engineering Frontiers of Engineering Symposia and delivered plenary lectures in that forum. He recently received the Harold E. Edgerton Faculty Achievement Award for exceptional distinction in teaching and in research or scholarship, the highest honor bestowed on young MIT faculty. In 2016, he received the Feynman Prize in Nanotechnology for his work on hierarchical materials, and was elected as a Fellow of the American Institute for Medical and Biological Engineering (AIMBE) and NANOSMAT Society.

Professor Buehler is a member of the editorial board of numerous international publications, including the Journal of the Royal Society Interface, Nanotechnology, and is Editor-In-Chief of BioNanoScience, a journal he co-founded. He is the founding Chair of the Biomechanics Committee at the Engineering Mechanics Institute of the American Society of Civil Engineers (ASCE), and a member of the U. S. National Committee on Biomechanics. He has chaired several international conferences in the area of materials science and engineering, nanotechnology, nanomedicine and biomechanics. Since 2016, he serves as the Editor in Chief of the Journal of the Mechanical Behavior of Biomedical Materials (JMBBM), and is a member of the Editorial Board of Biophysical Journal.

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