



PREDICTIVE MULTISCALE MATERIALS DESIGN

June 13–17, 2022 | professional.mit.edu/mmd | Instructor: Markus J. Buehler (email: mbuehler@mit.edu)

	MONDAY, JUNE 13	TUESDAY, JUNE 14	WEDNESDAY, JUNE 15	THURSDAY, JUNE 16	FRIDAY, JUNE 17
7:00–7:45 am	REGISTRATION				
8:00–9:30 am	Lecture 1: Introduction: Materials by Design, from Atoms to Structures, Advanced Computing to Manufacturing	Lecture 5: Materiomics: Fundamentals and Applications of Bioinspired Design by Categorization; Case Study: Molecular Mechanics of Viral Proteins <i>In-class 3D printing: setting up (various additive methods and integration with computing and computer vision)</i>	Lecture 7: Advanced Simulation Methods: Reactive Force Fields, Chemical Modeling, Quantum Training and Machine Learning, High-Throughput Material Screening (Materials Genome); Advanced Machine Learning Methods Applied to Materials Modeling and Design (Autoencoders, NLP, Transformer, Game Theory/GANs, Graph Neural Networks and Geometric Deep Learning)	Lecture 9: Performance of Materials in Extreme Conditions: Resilience, Stability, Catastrophic Failure: Connecting Experiment, Modeling and Theory Case Study: Molecular Mechanics and Earthquakes	Lecture 11: Materiomics Case Study III: Natural and Synthetic Spider Webs in 2D and 3D; Experiment, Modeling and Additive Manufacturing of Advanced Materials <i>Live dissection of a hierarchical spider web structure, neural network modeling (GAN and NLP), and structure generation</i>
9:30–9:45 am	COFFEE BREAK				
9:45 am–12:30 pm	Lecture 2: Hierarchical Materials and Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI): Nanoengineering Hierarchical Materials to Meet Industrial Needs	Lecture 6: Predictive Design: Multiscale Self-Assembly and Additive Manufacturing; Fundamentals, Implementation, and Examples <i>In-class design studio and 3D printing of optimized materials (continuum optimization and microstructural modeling)</i>	Lecture 8: Materiomics Case Study II: Modeling, Design, Manufacturing and Characterization of <i>De Novo</i> ; Hierarchical Composite Materials: Turning Weakness to Strength <i>In-class coding exercise: machine learning convolutional classifier development, cloud computing demonstration</i>	Lecture 10: Survey of Quantitative Multiscale Experimental Tools; Translational Paradigms; Modeling in Science, Art and Music and Cross-Disciplinary Synthesis, Category Theory <i>Vibrational material model live demonstration</i>	Lecture 12: Supercomputing Tools, Code and Software Architecture; Cloud Simulations, Big Data and Analytics, Machine Learning and AI, Neuromorphic Computing, Quantum Computing, Outlook
12:30–1:00 pm	LUNCH BREAK (ON YOUR OWN)				
1:00–2:30 pm	Lecture 3: Fundamentals of Computational Materials Science: Concepts, Implementation and Examples, Physics and Data-Driven Methods	Lab 1: Hands-On Molecular Modeling: From the Bottom Up (includes simulation case studies, data analysis, visualization)	Lab 2: Bioinspired Materials and Additive Manufacturing; <i>Hands-on Application of machine learning and AI in materials design, virtual and augmented reality (AR/VR)</i>	Materials Design Clinic 2: <i>Machine learning, data collection, feasibility. Working with problems shared by participants for real-world solutions.</i>	Lecture 13: Concluding Lecture: Future Opportunities; Group Discussion; Certificates
2:30–2:45 pm	COFFEE BREAK				
2:45–4:00 pm	Lecture 4: Introduction to Machine Learning Clinic; Materiomics Case Study I: Bio-Inspired Surface Engineering (Gecko Nanotechnology and Adhesion), Industrial Applications of Multiscale Modeling and AI in Materials Engineering	Lab 1 (cont'd): Interactive Case Studies (participants give short presentations, interactive discussion)	Lab 2 (cont'd): <i>Bioinspired Materials and Additive Manufacturing, Materials Processing Laboratory</i> (virtual interactive lab tour, videos, and live demo by the instructor) Materials Design Clinic 1	Lab 3: <i>Presentations and discussions, time for open Q&A (interactive group activity)</i>	Note: All times are US Eastern Daylight Time. Schedule is subject to change.
4:00–5:30 pm	RECEPTION (includes participant introductions) 1-236 (Spofford Room)	Optional: <i>Time for group work and assignments (can be arranged within groups at other times), instructor is available for personal meetings</i>	Optional: <i>Time for group work and assignments (can be arranged within groups at other times), instructor is available for personal meetings</i>		COLOR CODE Black font – Lecture activity <i>Bold italic font – Interactive work</i> In-class interactive simulations performed via in-browser cloud computing (access to internet via browser required)