PROFESSIONAL EDUCATION

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 ***In-class 3D printing: setting up (various additive methods and integration with computing and computer vision)***	**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 ***Live dissection of a hierarchical spider web structure, neural network modeling (GAN and NLP), and structure generation***
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 ***In-class design studio and 3D printing of optimized materials (continuum optimization and microstructural modeling)***	**Lecture 8:** Materiomics Case Study II: Modeling, Design, Manufacturing and Characterization of *De Novo*; Hierarchical Composite Materials: Turning Weakness to Strength ***In-class coding exercise: machine learning convolutional classifier development, cloud computing demonstration***	**Lecture 10:** Survey of Quantitative Multiscale Experimental Tools; Translational Paradigms; Modeling in Science, Art and Music and Cross-Disciplinary Synthesis, Category Theory ***Vibrational material model live demonstration***	**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)**				**Lecture 13:** Concluding Lecture: Future Opportunities; Group Discussion; Certificates
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; ***Hands-on Application of machine learning and AI in materials design, virtual and augmented reality (AR/VR)***	**Materials Design Clinic 2:** ***Machine learning, data collection, feasibility. Working with problems shared by participants for real-world solutions.***	**ADJOURN**
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):** ***Bioinspired Materials and Additive Manufacturing, Materials Processing Laboratory*** (virtual interactive lab tour, videos, and live demo by the instructor) **Materials Design Clinic 1**	**Lab 3:** ***Presentations and discussions, time for open Q&A (interactive group activity)***	Note: All times are US Eastern Daylight Time. Schedule is subject to change. **COLOR CODE** Black font – Lecture activity ***Bold italic font – Interactive work*** In-class interactive simulations performed via in-browser cloud computing (access to internet via browser required)
4:00–5:30 pm	**RECEPTION** (includes participant introductions) 1-236 (Spofford Room)	Optional: ***Time for group work and assignments (can be arranged within groups at other times), instructor is available for personal meetings***	Optional: ***Time for group work and assignments (can be arranged within groups at other times), instructor is available for personal meetings***		