PROFESSIONAL EDUCATION

PREDICTIVE MULTISCALE MATERIALS DESIGN

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

	MONDAY, JUNE 21	TUESDAY, JUNE 22	WEDNESDAY, JUNE 23	THURSDAY, JUNE 24	FRIDAY, JUNE 25
7:00–7:45 am	**REGISTRATION**				
8:00–9:30 am	Introduction: Materials by Design, from Atoms to Structures, Advanced Computing to Manufacturing **L1**	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)*** **L5**	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) **L7**	Performance of Materials in Extreme Conditions: Resilience, Stability, Catastrophic Failure: Connecting Experiment, Modeling and Theory Case study: Molecular mechanics and earthquakes **L9**	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*** **L11**
9:30–9:45 am	**COFFEE BREAK**				
9:45 am–12:30 pm	Hierarchical Materials & Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI): Nanoengineering hierarchical materials to meet industrial needs **L2**	Predictive Design: Multiscale Self-assembly & Additive Manufacturing; Fundamentals, Implementation, and Examples ***In-class design studio and 3D printing of optimized materials (continuum optimization and microstructural modeling)*** **L6**	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*** **L8**	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*** **L10**	Supercomputing Tools, Code and Software Architecture; Cloud Simulations, Big Data & Analytics, Machine Learning and AI, neuromorphic computing, quantum computing, outlook **L12**
12:30–1:00 pm	**LUNCH BREAK (ON YOUR OWN)**				Concluding Lecture: Future Opportunities; Group Discussion; Certificates **L13**
1:00–2:30 pm	Fundamentals of Computational Materials Science: Concepts, Implementation and Examples, Physics and Data-driven Methods **L3**	**LAB 1:** Hands-on Molecular Modeling: From the Bottom Up (includes simulation case studies, data analysis, visualization)	**LAB 2:** Bioinspired Materials & 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	Introduction to machine learning clinic; Materiomics Case Study I: Bio-inspired Surface Engineering (Gecko Nano-technology & Adhesion), industrial applications of multiscale modeling and AI in materials engineering **L4**	**LAB 1 (cont'd):** Interactive Case Studies (participants give short presentations, interactive discussion)	**LAB 2 (cont'd):** ***Bioinspired Materials & 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.
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***		**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)