PROFESSIONAL EDUCATION | LIVE Virtual

PREDICTIVE MULTISCALE MATERIALS DESIGN SHORT COURSE

JUNE 21–25, 2021 | Instructor: Markus J. Buehler (email: mbuehler@mit.edu)

Note: All times are US Eastern Daylight Time. Schedule is subject to change.

	MONDAY, JUNE 21	TUESDAY, JUNE 22	WEDNESDAY, JUNE 23	THURSDAY, JUNE 24	FRIDAY, JUNE 25
8–9:30 am	L1 Introduction: Materials by Design, from Atoms to Structures, Advanced Computing to Manufacturing	L5 Materiomics: Fundamentals and Applications of Bioinspired Design by Categorization Case study: Molecular mechanics of viral proteins ***In-class 3D printing – setting up (various methods)***	L7 Advanced Simulation Methods: Reactive Force Fields, Chemical Modeling, Quantum Training and Machine Learning	L9 Performance of Materials in Extreme Conditions: Resilience, Stability, Catastrophic Failure: Connecting Experiment, Modeling and Theory Case study: Molecular mechanics and earthquakes	L11 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 and structure generation***
9:30-9:45 am	**BREAK**	**BREAK**	**BREAK**	**BREAK**	**BREAK**
9:45 am–12:30 pm	L2 Hierarchical Materials & Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI)	L6 Predictive Design: Multiscale Self-assembly & Additive Manufacturing; Fundamentals, Implementation, and Examples ***In-class design studio and 3D printing of optimized materials***	L8 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 classifier development***	L10 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***	L12 Supercomputing Tools, Code and Software Architecture; Cloud Simulations, Big Data & Analytics, Machine Learning and AI, neuromorphic computing, quantum computing, outlook
12:30–1:00 pm	**LUNCH (on your own)**	**LUNCH (on your own)**	**LUNCH (on your own)**	**LUNCH (on your own)**	L13 Concluding Lecture: Future Opportunities; Group Discussion ***Certificates***
1:00–2:30 pm	L3 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 INTRO LECTURE: Bioinspired Materials & Additive Manufacturing ***Hands-on Application of Machine Learning and AI in Materials Design***	LAB 3: ***Participants work on Group Assignments (work done in groups, in Zoom breakout rooms, mentored by the instructor)***	Adjourn
2:30–2:45 pm	**BREAK**	**BREAK**	**BREAK**	**BREAK**	
2:45–4 pm	Materiomics Case Study I: Bio-inspired Surface Engineering (Gecko Nanotechnology & Adhesion)	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)***	LAB 3 (cont'd): ***Presentations and Discussions, time for open Q&A (interactive group activity)***	**KEY:** Regular font = Lecture activity ***Bold, italic font = Interactive work*** In-class interactive simulations performed via in-browser cloud computing (access to internet via browser required)
4–5:30 pm	VIRTUAL 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 Zoom sessions***	Optional: ***Time for Group Work and Assignments (can be arranged within groups at other times); Instructor is available for personal Zoom sessions***		