

# Schedule – Predictive Multiscale Materials Design Short Course 2020

Instructor: Markus J. Buehler (email: [mbuehler@MIT.EDU](mailto:mbuehler@MIT.EDU)). *This course will be delivered in a live virtual format.*

Time	Monday 6/1	Tuesday 6/2	Wednesday 6/3	Thursday 6/4	Friday 6/5
8-8:45 am	<b>REGISTRATION</b>				
9-10:15 am	Introduction: Materials by Design, from Atoms to Structures, Advanced Computing to Manufacturing <b>L1</b>	Materiomics: Fundamentals and Applications of Bioinspired Design by Categorization <b>L5</b>	Advanced Simulation Methods: Reactive Force Fields, Chemical Modeling, Quantum Training and Machine Learning <b>L7</b>	Performance of Materials in Extreme Conditions: Resilience, Stability, Catastrophic Failure: Connecting Experiment, Modeling and Theory <b>L9</b>	Materiomics Case Study III: Natural and Synthetic Spider Webs in 2D and 3D; Experiment, Modeling and Additive Manufacturing of Advanced Materials <b>L11</b>
10:15-10:30 am	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>
10:30-noon:	Hierarchical Materials & Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI) <b>L2</b>	Predictive Design: Multiscale Self-assembly & Additive Manufacturing; Fundamentals, Implementation, and Examples <b>L6</b>	Materiomics Case Study II: Modeling, Design, Manufacturing and Characterization of <i>De Novo</i> Hierarchical Composite Materials <b>L8</b>	Survey of Quantitative Multiscale Experimental Tools; Translational paradigms; Modeling in Science, Art and Music and Cross-disciplinary Synthesis <b>L10</b>	Supercomputing Tools, Code and Software Architecture; Cloud Simulations, Big Data & Analytics, Machine Learning and AI, Outlook <b>L12</b>
12:00-1:00 pm	<b>LUNCH (on your own)</b>	<b>LUNCH (on your own)</b>	<b>LUNCH (on your own)</b>	<b>LUNCH (on your own)</b>	Concluding Lecture, Future Opportunities Group Discussion; Certificates <b>L13</b>
1:00-3:00 pm	Fundamentals of Computational Materials Science: Concepts, Implementation and Examples, Physics and Data-driven Methods <b>L3</b>	<b>LAB LECTURE 1:</b> Hands-on Molecular Modeling – From the Bottom Up (includes simulation case studies, data analysis, visualization)	<b>LAB LECTURE 2</b> INTRO LECTURE: Bioinspired Materials & Additive Manufacturing; Hands-on Application of Machine Learning and AI in Materials Design	<b>LAB 3:</b> Participants work on Group Assignments (work done in groups, in the classroom, mentored by the instructor)	<i>Adjourn</i>
3:00-3:15 pm	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	<b>COFFEE BREAK</b>	
3:15-5 pm	Materiomics Case Study I: Bio-inspired Surface Engineering (Gecko Nanotechnology & Adhesion) <b>L4</b>	<b>LAB 1:</b> Interactive Case Studies (participants give short presentations, interactive discussion)	<b>LAB 2:</b> Bioinspired Materials & Additive Manufacturing, Materials Processing Laboratory (virtual lab tour, videos, and live demo by the instructor)	<b>LAB 3 (cont'd):</b> Presentations and Discussions, time for open Q&A (interactive group activity)	