

Schedule – Predictive Multiscale Materials Design Short Course 2020

Instructor: Markus J. Buehler

Time	Monday 6/1	Tuesday 6/2	Wednesday 6/3	Thursday 6/4	Friday 6/5
8-8:45 am	REGISTRATION				
9-10:15 am	Introduction: Materials by Design, from Atoms to Structures, Advanced Computing to Manufacturing L1	Materiomics: Fundamentals and Applications of Bioinspired Design by Categorization L5	Advanced Simulation Methods: Reactive Force Fields, Chemical Modeling, Quantum Training and Machine Learning L7	Performance of Materials in Extreme Conditions: Resilience, Stability, Catastrophic Failure: Examples of Connecting Experiment, Modeling and Theory L9	Materiomics Case Study III: Natural and Synthetic Spider Webs in 2D and 3D; Experiment, Modeling and Additive Manufacturing of Advanced Materials L11
10:15-10:30 am	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK
10:30-noon:	Hierarchical Materials & Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI) L2	Predictive Design: Multiscale Self-assembly & Additive Manufacturing; Fundamentals, Implementation, and Examples L6	Materiomics Case Study II: Modeling, Design, Manufacturing and Characterization of <i>De Novo</i> Hierarchical Composite Materials L8	Survey of Quantitative Multiscale Experimental Tools; Translational paradigms; Modeling in Science, Art and Music and Cross-disciplinary Synthesis L10	Supercomputing Tools, Code and Software Architecture; Cloud Simulations, Big Data & Analytics, Machine Learning and AI, Outlook L12
12:00-1:00 pm	LUNCH (on your own)	LUNCH (on your own)	LUNCH (on your own)	LUNCH (on your own)	Concluding Lecture, Future Opportunities Group Discussion; Certificates L13
1:00-3:00 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 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 the classroom, mentored by the instructor)	<i>Adjourn</i>
3:00-3:15 pm	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	
3:15-5 pm	Materiomics Case Study I: Bio-inspired Surface Engineering (Gecko Nanotechnology & Adhesion) L4	Interactive Case Studies (participants give short presentations, interactive discussion)	LAB 2 (cont'd): Bioinspired Materials & Additive Manufacturing, Materials Processing Laboratory	LAB 3 (cont'd): Presentations and Discussions, time for open Q&A (interactive group activity)	
5-6:30 pm	RECEPTION (all participants and instructor – includes introductions) 1-236 (Spofford Room)	Optional: Time for Group Work and Assignments	Optional: Time for Group Work and Assignments		