Schedule – Predictive Multiscale Materials Design Short Course 2021

Instructor: Markus J. Buehler

Time	Monday June 21	Tuesday June 22	Wednesday June 23	Thursday June 24	Friday June 25
7-7:45 am	**REGISTRATION**				
8-9:30 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 methods) **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: 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 and structure generation **L11**
9:30-9:45 am	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**
9:45-12:30:	Hierarchical Materials & Structures: Biological Design, Feynman Paradigm and Artificial Intelligence (AI) **L2**	Predictive Design: Multiscale Self-assembly & Additive Manufacturing; Fundamentals, Implementation, and Examples In-class design studio and 3D printing of optimized materials **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 classifier development **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 (on your own)**	**LUNCH (on your own)**	**LUNCH (on your own)**	**LUNCH (on your own)**	Concluding Lecture: Future Opportunities Group Discussion; Certificates **L13**
1:00-2:30 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** 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	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	
2:45-4 pm	Materiomics Case Study I: Bio-inspired Surface Engineering (Gecko Nanotechnology & Adhesion) **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)	**LAB 3 (cont'd):** Presentations and Discussions, time for open Q&A (interactive group activity)	
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		

Color code: Black font – lecture activity, blue font – interactive work

In-class interactive simulations performed via in-browser cloud computing (access to internet via browser required)