TITLE: Bioinspired Artificial Intelligence and Biomaterials by Design

### SPEAKER: Markus J. Buehler

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#### Abstract

Nature produces a variety of materials with many functions, often out of simple and abundant materials, and at low energy. Such systems - examples of which include silk, tendon, bone, nacre or diatoms - provide broad inspiration for engineering. Here we explore the translation of biological composites to engineering applications, using a variety of tools including molecular modeling, AI and machine learning, and experimental synthesis and characterization. We review a series of studies focused on the mechanical behavior of materials, especially deformation and fracture, and how these phenomena can be modeled using a combination of molecular dynamics and machine learning, to generate a novel simulated evolutionary process that offers directed adaptation of biomaterial properties. We also present various case studies of material optimization using genetic algorithms, applied to 3D printed composites, protein design, and a translation of protein folding to music and back. We also review a close integration of music and materials and review our recent research on a new bio-inspired compositional technique called materiomusic.

## Bio

Markus J. Buehler is the McAfee Professor of Engineering at MIT, a member of the Center for Materials Science and Engineering, and the Center for Computational Science and Engineering at the Schwarzman College of Computing. In his research, Professor Buehler pursues new modeling, design and manufacturing approaches for advanced biomaterials that offer greater resilience and a wide range of controllable properties from the nano- to the macroscale. His interests include a variety of functional material properties including mechanical, optical and biological, linking chemical features, hierarchical and multiscale structures, to assessments of material performance in the context of physiological, pathological and other extreme conditions. His methods include molecular and multiscale modeling, AI, and ML, as well as experimental synthesis and characterization. His particular interest lies in the mechanics of complex hierarchical materials with features across scales (e.g. nanotubes, graphene, and natural biomaterial nanostructures, especially protein materials).

His research has had broad impact, and resulted in a new paradigm for the analysis of bioinspired materials and structures to devise new biomaterial platforms, and using a mathematical categorization approach that connects insights from disparate fields such as materials, structures to music and language. His research has been seminal in the introduction of AI methods in materials modeling of mechanical properties, especially fracture mechanics, composites, and 3D printing, featuring a novel perspective to connect datasets form experiment and simulation to develop multiscale models of mechanical systems. He has applied these methods to wide ranging areas of application including protein folding, fracture, and composite design, and coupled the de novo design methods with additive manufacturing approaches. He is well-known for his research on mechanically relevant proteins, especially silk, elastin, intermediate filaments, and collagen. Buehler has authored more than 450 peer-reviewed publications (H-index=92), which have been cited more than 30,000 times, and authored two monographs (as well as several edited books). He has given more than 400 invited, keynote and plenary talks around the world, and given several highly praised TED talks. His technical innovations have resulted in several patents.

He is the Editor-in-Chief of the Journal of the Mechanical Behavior of Biomedical Materials and is active on the editorial board of many other peer-reviewed journals. Buehler is an elected member of the Board of Directors of the Society of Engineering Science (SES), and between 2018 and 2020 served a three-year term as President-elect, President and Past President of SES. He served as the chair of several conferences, various societal committees in professional organizations, and is actively involved in public outreach (including an annual materials research camp at MIT with local middle and high schools). From 2013-2020 he served as the Head of the Civil and Environmental Engineering Department at MIT. During his tenure he led renewal of the department with a new vision at the nexus of environment and infrastructure that resulted in renewal of around one third of the department's faculty, substantial increases in the national and global rankings, a significant increase of faculty diversity, and extensive space renovations.

He is the recipient of many awards including the Harold E. Edgerton Faculty Achievement Award, the Alfred Noble Prize, the Feynman Prize in Nanotechnology, the Leonardo da Vinci Award, and the Thomas J.R. Hughes Young Investigator Award, and others. He is a recipient of the National Science Foundation CAREER award, the United States Air Force Young Investigator Award, the Navy Young Investigator Award, and the Defense Advanced Research Projects Agency (DARPA) Young Faculty Award, as well as the Presidential Early Career Award for Scientists and Engineers (PECASE). In 2016 he was awarded the Foresight Institute Feynman Prize for his advances in nanotechnology. He was named highly cited researcher by the Royal Society of Chemistry and awarded the Materials Horizons -Outstanding Paper Prize. In 2018, he was selected as a Clarivate Highly Cited Researcher, for his sustained high-impact contributions to scholarship recognizing exceptional research performance demonstrated by production of multiple highly cited papers that rank in the top 1% by citations. In 2020, he was named as one of the global top 0.09% of all researchers, worldwide, in the nanoscience/materials category in a study from Stanford University.

In addition to his regular undergraduate and graduate teaching at MIT, Buehler offers an annual Professional Education course "Predictive Multiscale Materials Design". As an active composer of classical and experimental music, he is deeply involved in scientific outreach and the intersection of art and science, and a member of the Executive Committee of MIT's Center for Art, Science and Technology (CAST). Based on his record in the translation of basic research into practice through entrep reneurship, he is heavily involved with start-ups and innovation, such as through his role on the Board of Directors of Sweetwater Energy, Inc. and as a member of the Scientific Advisor Board of Safar Partners (A Technology Venture Fund with Private Equity Vision). He has extensive experience in scientific and engineering consulting for industry and practice.