Markus J. Buehler, Ph.D. Mechanical Engineering & Civil and Environmental Engineering McAfee Professor of Engineering Massachusetts Institute of Technology Director and PI, Laboratory for Atomistic and Molecular Mechanics (LAMM) Lab URL: <u>http://lamm.mit.edu/</u> Personal website: <u>https://meche.mit.edu/people/faculty/mbuehler@mit.edu</u> <u>mbuehler@MIT.EDU</u>

EXECUTIVE SUMMARY: Markus J. Buehler is the McAfee Professor of Engineering at MIT, an Institute-wide Endowed Chair, a member of the Center for Materials Science and Engineering, as well as the Center for Computational Science and Engineering at MIT's Schwarzman College of Computing. He holds academic appointments in both Mechanical Engineering and Civil and Environmental Engineering.

In his research, Professor Buehler develops innovative modeling, design, and manufacturing approaches for advanced biomaterials, emphasizing resilience and a broad spectrum of controllable properties from the nano- to the macroscale. His work spans various functional material properties, including mechanical, optical, and biological, linking chemical features and hierarchical and multiscale structures to performance under physiological, pathological, and other extreme conditions, with a particular focus on materials failure. Professor Buehler's methodologies incorporate molecular and multiscale modeling, AI and deep learning, design, and experimental synthesis and characterization. He has pioneered the use of multi-agent AI systems for scientific problem-solving and discovery, as well as graph reasoning strategies based on category theory. His work resulted in the discovery of size effects governing the mechanics of structural proteins as found in silk, collagen and elastin, as well as methods to design *de novo* proteins and biomaterials for novel mechanical properties.

From 2013 to 2020, Buehler served as Department Head of MIT's Civil and Environmental Engineering Department, where he hired one-third of the department's faculty, significantly shaping its direction and strategic focus, as well as developing new educational programs. He has held numerous leadership roles in professional organizations, including a term as President of the Society of Engineering Science (SES) and as Editor in Chief of the Journal of the Mechanical Behavior of Biomedical Materials, among others. Buehler is a member of the National Academy of Engineering.

Institution	Major	Degree & Year
University of Stuttgart Stuttgart, Germany	Process and Chemical Engineering	Pre-Diploma (B.S. eq.), 2000
Michigan Technological University Houghton, Michigan	Engineering Mechanics	M.S., 2001
Max Planck Institute for Metals Research University of Stuttgart Stuttgart, Germany	Chemistry (Materials Science)	Dr. rer. nat. (Ph.D.), 2004
California Institute of Technology Pasadena, California	Chemistry and Chemical Engineering	Postdoctoral Scholar, 2004-2005
Massachusetts Institute of Technology Cambridge, Massachusetts	Civil and Environmental Engineering	Postdoctoral Associate 2005-2006

PROFESSIONAL TRAINING

PROFESSIONAL APPOINTMENTS

2021 - present	Professor, Mechanical Engineering, MIT
2019	President, Society for Engineering Science (SES)
2018-present	Safar Partners Equity Fund, Scientific Advisory Board
2017-2023	Member of the Board of Directors, Sweetwater Energy, Inc.
2015-present	McAfee Professor of Engineering (Institute-wide Endowed Chair Professorship), MIT
2013-2020	Head of Department, Dept. Civil and Environmental Engineering, MIT
2013-present	Professor (with tenure), Dept. Civil and Environmental Engineering, MIT
2011-2013	Co-Director, MIT Computation for Design and Optimization Program
2011-2013	Associate Professor with Tenure, Dept. Civil and Environmental Engineering, MIT
2010-2013	Group Leader, Mechanics and Materials Division in Civil & Environmental Engineering, MIT
2010-2023	Director, MIT-Germany Program, MIT
2009-2010	Esther and Harold Edgerton Associate Professor, Civil and Environmental Engineering, MIT 2007-
2009	Esther and Harold Edgerton Assistant Professor, Civil and Environmental Engineering, MIT 2006-
2007	Assistant Professor, Dept. Civil and Environmental Engineering, MIT
2005-2006	Lecturer and Postdoctoral Associate, MIT
2004-2005	Director of Multiscale Modeling and Software Integration, Materials and Process Simulation
	Center, California Institute of Technology, Pasadena

2004-2005	Postdoctoral Scholar, California Institute of Technology, Pasadena
2004	Postdoctoral Fellow, Max Planck Institute for Metals Research, Stuttgart, Germany
2001-2004	Research Assistant, Max Planck Institute for Metals Research, Stuttgart, Germany
2001	Internship at Robert Bosch GmbH, Plastics Engineering. Waiblingen, Germany
2000-2001	Graduate Research Assistant, Department of Mechanical Engineering-Engineering Mechanics,
	Michigan Technological University

<u>PEER-REVIEWED PUBPLICATIONS</u>: Total: 500+ peer reviewed articles, several books and book chapters; H-index 116 (Google Scholar), 49,000+ citations, Clarivate Highly Cited Researcher. Full list of publications at: <u>https://scholar.google.com/citations?user=hWBTSksAAAJ&hl=en</u>

Selection of Key publications

- 1. B. Ni, M.J. Buehler, MechAgents: Large language model multi-agent collaborations can solve mechanics problems, generate new data, and integrate knowledge, *Extreme Mechanics Letters*, Vol. 67, 102131, 2024.
- 2. M.J. Buehler, Cephalo: Multi-Modal Vision-Language Models for Bio-Inspired Materials Analysis and Design, arXiv <u>https://arxiv.org/abs/2405.19076</u>, 2024.
- 3. M.J. Buehler, Accelerating Scientific Discovery with Generative Knowledge Extraction, Graph-Based Representation, and Multimodal Intelligent Graph Reasoning, arXiv <u>https://arxiv.org/abs/2403.11996</u>, 2024.
- 4. S.C. Shen, N.A. Lee, W.J. Lockett, A.D. Acuil, H.B. Gazdus, B.N. Spitzer, M.J. Buehler, Robust myco-composites: a biocomposite platform for versatile hybrid-living materials, *Mat. Horiz.*, 11, 1689-1703, 2024.
- M.J. Buehler, MechGPT, a Language-Based Strategy for Mechanics and Materials Modeling That Connects Knowledge Across Scales, Disciplines, and Modalities, *ASME Appl. Mech. Rev.*, 76(2): 021001, https://doi.org/10.1115/1.4063843, 2024.
- E.L. Buehler, M.J. Buehler, X-LoRA: Mixture of Low-Rank Adapter Experts, a Flexible Framework for Large Language Models with Applications in Protein Mechanics and Design, *APL Mach. Learn.* 2, 026119, https://doi.org/10.1063/5.0203126, 2024.
- 7. A. Lew, M.J. Buehler, "Single-shot forward and inverse hierarchical architected materials design for nonlinear mechanical properties using an attention-diffusion model," *Mater. Tod.*, 2023, 10.1016/j.mattod.2023.03.007, 2023.
- 8. M. Buehler, "Unsupervised cross-domain translation via deep learning and adversarial attention neural networks and application to music-inspired protein designs," *Patterns*, 2023, 10.1016/j.patter.2023.100692.
- 9. R. Luu and M.J. Buehler, BioinspiredLLM: Conversational Large Language Model for the Mechanics of Biological and Bio-Inspired Materials, *Adv. Sci.*, <u>https://doi.org/10.1002/advs.202306724</u>, 2023.
- 10. F. Liu, B. Ni, M.J. Buehler, "PRESTO: Rapid protein mechanical strength prediction with an end-to-end deep learning model," *Extreme Mechanics Letters*, paper # 101803, 2022
- 11. Z. Yang, M.J. Buehler, "High-Throughput Generation of 3D Graphene Metamaterials and Property Quantification Using Machine Learning," *Small Methods*, paper # 2200537, 2022
- 12. A.J. Lew, M.J. Buehler, "DeepBuckle: Extracting physical behavior directly from empirical observation for a material agnostic approach to analyze and predict buckling," *JMPS*, Vol. 164, 103909, 2022
- 13. Z. Yang, C.-H. Yu, M.J. Buehler, "Deep Learning Model to Predict Complex Stress and Strain Fields in Hierarchical Composites," *Science Advances*, DOI: 10.1126/sciadv.abd7416, 2021
- 14. K. Guo, M.J. Buehler, "A semi-supervised approach to architected materials design using graph neural networks," *Extreme Mechanics Letters*, Vol. 41, pp. 101029, 2020
- 15. M.J. Buehler, "Liquified protein vibrations, classification and cross-paradigm *de novo* image generation using deep neural networks," *Nano Futures*, p. 035004, Vol. 4(3), 2020
- 16. M. Hsu, C.H. Yu, M.J. Buehler, "Using Deep Learning to Predict Fracture Patterns in Crystalline Solids," *Cell Matter*, Vol. 3, 1-15, 2020
- 17. C.H. Yu; M.J. Buehler, "Sonification based de novo protein design using artificial intelligence, structure prediction, and analysis using molecular modeling," *APL Bioengineering*, Vol. 4(1), p. 016108, 2020.
- 18. D. Liu, A. Tarakanova, C. C. Hsu, M. Yu, S. Zheng, L. Yu, J. Liu, Y. He, D. J. Dunstan, and M. J. Buehler, "Spider dragline silk as torsional actuator driven by humidity," *Science Adv.*, Vol. 5, no. 3, 2019
- 19. G.X. Gu, C.-T. Chen, M.J. Buehler "*De novo* composite design based on machine learning algorithm", *Extreme Mechanics Letters* 18, p. 19-28, 2018
- G. X. Gu, C.-T. Chen, D. J. Richmond, and M. J. Buehler, "Bioinspired hierarchical composite design using machine learning: simulation, additive manufacturing, and experiment," *Mater. Horizons*, vol. 5, no. 5, pp. 939–945, Aug. 2018 (Selected as 2018 Outstanding Paper Prize winner)
- 21. S. Ling; Z. Qin; W. Huang; S. Cao; D. L. Kaplan; M. J. Buehler, "Design and function of biomimetic multilayer water purification membranes," *Science Adv.*, DOI: 10.1126/sciadv.1601939, 3 (4), e1601939, 2017 (the technology to develop filtration devices from silk, protein and hybrid nanofibrillar materials has been covered in a series of patents)
- 22. C.C. Chou, M.J. Buehler, Structure and Mechanical Properties of Human Trichocyte Keratin Intermediate Filament Protein, *Biomacromolecules*, Vol. 13(11), 3522-3532, 2012.
- 23. S. Keten, Z. Xu, B. Ihle, M.J. Buehler, "Nanoconfinement controls stiffness, strength and mechanical toughness of beta-sheet crystals in silk," *Nature Materials* Vol. 9, 359-367, 2010

- 24. Z. Xu, R. Paparcone, M.J. Buehler, "Alzheimer's Aβ(1-40) amyloid fibrils feature size dependent mechanical properties," *Biophysical Journal* Vol 98(10), 2053-2062, 2010.
- 25. Buehler, M.J., "Nature designs tough collagen: Explaining the nanostructure of collagen fibrils," Proc. Nat'l Academy of Sciences USA 103(33), 12285-12290, 2006

Other publications

- 1. E. Khare, N. Holten-Andersen, M.J. Buehler, "Transition metal-coordinate bonds in protein-inspired materials and engineered polymer hydrogels for tunable mechanical properties," *Nature Reviews Materials*, DOI: 10.1038/s41578-020-00270-z, 2021
- T. Sapra, Z Qin, A. Dubrokvsky-Gaupp, U. Aebi, D. Muller, M.J. Buehler, O. Medala, "Nonlinear mechanics of lamin filaments and the meshwork topology build an emergent nuclear lamina," *Nature Communications*, DOI: https://doi.org/10.1101/846550, 2020
- 3. I. Su, M.J. Buehler, "Mesomechanics of a Three-Dimensional Spider Web," *Journal of the Mechanics and Physics of Solids*, Vol. 144, p. 104096, 2020
- 4. W. S. Leong, H. Wang, J. Yeo, F. J. Martin-Martinez, A. Zubair, P.-C. Shen, Y. Mao, T. Palacios, M. J. Buehler, J.-Y. Hong, and J. Kong, "Paraffin-enabled graphene transfer," *Nat. Commun.*, Vol. 10, p. 867, 2019.
- 5. J. Yeo; G. Jung; F. Martin-Martinez; J. Beem; Z. Qin; M. Buehler, "Multiscale design of graphyne-based materials for high-performance separation membranes," *Advanced Materials*, https://doi.org/10.1002/adma.201805665, 2019
- 6. E. Beniash, C. Stifler, C.-Y. Sun, G.S. Jung, Z. Qin, M.J. Buehler, P. Gilbert, "The hidden structure of human enamel," *Nature Communications*, paper #: 4383, 2019
- 7. Y. Han, M. Li, G. Jung, M. A. Marsalis, Z. Qin, M. J. Buehler, L. Li, D. A. Muller "Sub-nanometre channels embedded in two-dimensional materials" *Nature Materials* (cover article), Vol. 17.2, pp. 129-133, 2018
- 8. Z. Qin, G.S. Jung, M.J. Kang, M.J. Buehler, "The mechanics and design of a lightweight three-dimensional graphene assembly," *Science Advances* 3 (1), e1601536SD, 2017
- 9. S.J. Ling; C.M. Li; K. Jin; D.L. Kaplan; M.J. Buehler, "Liquid Exfoliated Natural Silk Nanofibrils: Applications in Optical and Electrical Devices," *Advanced Materials*, 28 (35), pp. 7783, 2016
- 10. S.W. Cranford, A. Tarakanova, N. Pugno, M.J. Buehler, "Nonlinear constitutive behaviour of spider silk minimizes damage and begets web robustness from the molecules up," *Nature*, Vol. 482, pp. 72-76, 2012 (cover article)
- 11. D. Sen, K. Novoselov, P. Reis and M.J. Buehler, "Tearing of graphene sheets from adhesive substrates produces tapered nanoribbons," *Small* 6(10), 1108-1116, 2010 (cover article).
- 12. R. Ritchie, M.J. Buehler, P. Hansma, "Plasticity and toughness of bone," Physics Today 62(6), 41-47, 2009.
- Ackbarow, T., X. Cheng, S. Keten and M.J. Buehler, "Hierarchies, multiple energy barriers and robustness govern the fracture mechanics of alpha-helical proteins," Proc. Nat'l Academy of Sciences USA 104(42), 16410-16415, 2007
- 14. Buehler, M.J., H. Tang, A. C.T. van Duin, W.A. Goddard III, "Threshold Crack Speed Controls Dynamical Fracture of Silicon Single Crystals," *Physical Review Letters*, 99, 165502, 2007
- 15. M.J. Buehler and H. Gao, "Dynamical fracture instabilities due to local hyperelasticity at crack tips," *Nature*, Vol. 439, pp. 307-310, 2006

OTHER ACTIVITIES, SERVICE AND LEADERSHIP

1. Invited, Keynote and Plenary Talks:

More than 500 invited talks, including many plenary and keynote lectures given around the world, at major conferences, workshops, and various research institutions and industry. His set of presentations also includes several TED talks and broad-impact general audience lectures.

2. Editorial Activities:

Editor-in-Chief, J. Mech. Behav. Biomed. Mat. (Elsevier); Section Editor, MRS Bulletin Impact; Editor-in- Chief, BioNanoScience (Springer); Cell Matter, Member of the Editorial Advisory Board (Cell Press); Editorial Advisory Board, ACS Biomaterials Science and Engineering (American Chemical Society); Proceedings of the National Academy of Sciences (PNAS), Handling Editor; Editorial Board Member, Extreme Mechanics Letters (Elsevier); Editor Board Member, Scientific Reports (Nature Publishing Group); Editorial Board, Computational Materials Science (Elsevier); Academic Editor, PLoS ONE (Public Library of Science); Associate Editorial Board, Frontiers in Mechanics of Materials (Frontiers); Guest Editor, MRS Bulletin (MRS); Executive Editor, International Journal of Applied Mechanics (Imperial College Press); Associate Editor, Journal of Engineering Mechanics (ASCE); Editorial Board, Journal of Nanomechanics and Micromechanics (ASCE); Associate Editor,

J. Comp. Theor. Nanosci. (Amer. Sci. Publ.); Editor, Acta Mech. Sinica (Springer Nature); Guest Editor of J. Mater. Res. (Springer Nature).

3. Committees and Service (selection)

MIT Committee on Arts, Culture, and DEI, 2021-2022; Chair, MRS Fall 2021 Meeting, 2019-2021; Member, Core Committee of New Engineering Education Transformation (NEET), MIT, 2017-2019; MIT Refugee ACTion (ReACT) Senior Advisory Committee, 2017- now; MIT Center for Computational Engineering Advisory Council, 2019-now; 2018-19, Co-Chair Eighth International Conference on Mechanics of Biomaterials & Tissues; Member of

the Executive Committee, ASME Materials Division (2015-2018); Co-Chair, NanoEngineering in Medicine and Biology (NEMB) Congress 2013, Boston, 2013; Chair, Fourth International Conference on Mechanics of Biomaterials & Tissues 2011, Hawai'i; Inaugural Chair, Biomechanics Committee at the ASCE Engineering Mechanics Institute (EMI), 2008-2014; Co-Chair, NanoEngineering for Medicine & Biology Congress Steering Committee of ASME, 2010-2013; Member, ASME Nanoengineering Council Executive Committee, 2010.

4. Teaching

- 3.021J Introduction to Modeling and Simulation (undergraduate)
- 1.545 Atomistic Modeling and Simulation of Materials (graduate)
- 1.050 Engineering Mechanics (undergraduate)
- 1.052/1.121/2.169 Advancing Mechanics and Materials via Machine Learning (graduate & undergraduate)
- "Predictive Multiscale Materials Design," MIT Professional Education short course (first offered in 2013, annual since then; with 200+ practicing engineering, science and technology professionals from around the world
- "Machine Learning for Materials Informatics," MIT Professional Education short course (since 2022)
- Co-instructor, "Machine Learning, Modeling, and Simulation: Engineering Problem-Solving in the Age of AI," MIT Professional & Executive Learning

HONORS AND AWARDS (selection of major awards)

- Elected Member, National Academy of Engineering, 2023
- Society of Engineering Science (SES) James R. Rice Medal, 2022
- International Association for Computational Mechanics (IACM) Fellows Award, 2022
- ASME Daniel C. Drucker Medal, 2021
- Royal Society of Chemistry Materials Horizons Outstanding Paper Prize, 2019
- MIT Distinguished Service and Leadership Award, 2021
- Clarivate Analytics Highly Cited Researcher Award, 2018 (recognized for exceptional research performance demonstrated by production of multiple highly cited papers that rank in the top 1% by citations for field and year in Web of Science)
- Feynman Prize (Foresight Institute), Theory, 2016
- Outstanding Young Scientist Award, NANOSMAT Society, 2016
- Fellow, NANOSMAT Society, 2016
- International Journal of Applied Mechanics (IJAM) Most Cited Paper Award (2009-2015), 2016
- Fellow, American Institute for Medical and Biological Engineering (AIMBE), 2015
- ASME Journal of Applied Mechanics Award 2014 (with student Zhao Qin)
- The Minerals, Metals & Materials Society (TMS) Robert Lansing Hardy Award, 2013
- NAE Frontiers of Engineering: Plenary Speaker, 2008 and 2013; Invited Participant, 2007
- TMS Structural Materials Division Best Paper Award 2013
- Materials Research Society (MRS) Outstanding Young Investigator Award, 2012
- IEEE Holm Conference Morton Antler Lecture Award, 2012
- SES Young Investigator Medal, 2012
- Alfred Noble Prize, 2011
- ASME Thomas J.R. Hughes Young Investigator Award, 2011
- ASCE Leonardo Da Vinci Award, 2011
- Stephen Brunauer Award, 2011 (American Ceramic Society)
- AIME Rossiter W. Raymond Memorial Award, 2011
- ASME Sia Nemat Nasser Award, 2010
- MIT Harold E. Edgerton Faculty Achievement Award, 2010
- Presidential Early Career Award for Scientists and Engineers (PECASE), 2009 (the award was presented by President Barack Obama at the White House)
- United States Navy Young Investigator Award, 2008
- DARPA Young Faculty Award, 2008
- Air Force Office of Scientific Research Young Investigator Award, 2008
- National Science Foundation CAREER Award, 2007
- Materials Research Society Gold Graduate Student Award, 2004

STUDENTS AND POSTDOCS

Graduated more than 45 PhD students and postdocs. Trained 90+ undergraduate and other researchers from programs at MIT (e.g. UROP), Research Science Institute (RSI) - Center for Excellence in Education, MIT MSRP, NSF-REU, and others. Many of his former students are now graduate students at major universities, hold faculty appointments at top universities around the world (Northwestern University, Berkeley University, Tsinghua University, KAIST, University College London, King's College London, and others), or hold high-profile jobs in industry or other leading organizations.