

Frontiers of Metastable Materials Development Using Artificial Intelligence: A Workshop

Committee

Raymundo Arroyave

Co-Chair

RAYMUNDO ARRÓYAVE is the Segers Family Dean's Excellence Professor, Presidential Impact Fellow, and Chancellor EDGES Fellow at Texas A&M University, where he serves as a professor in the Department of Materials Science and Engineering with joint appointments in Mechanical and Industrial & Systems Engineering. Arróyave's research focuses on computational materials science, integrating thermodynamics, kinetics, and artificial intelligence to accelerate the discovery and design of advanced materials for extreme environments. Arróyave is a fellow of ASM International and has received numerous distinctions, including the Acta Materialia Silver Medal (2023), TMS Brinacombe medal (2019), and NSF CAREER Award (2010) and his work has produced over 300 peer-reviewed publications and multiple patents. Arróyave earned his B.S. in Mechanical and Electrical Engineering from the Instituto Tecnológico y de Estudios Superiores de Monterrey and his MS and PhD in Materials Science and Engineering from the Massachusetts Institute of Technology.

Maria K. Chan

Co-Chair

MARIA K. CHAN is a scientist at the Center for Nanoscale Materials at Argonne National Laboratory, a senior fellow at the Northwestern Argonne Institute for Science and Engineering, and a fellow of the University of Chicago Consortium for Advanced Science and Engineering. Chan's research focuses on nanomaterials for energy applications, including solar cells, batteries, thermoelectrics, and catalysts with a particular focus on using artificial intelligence for efficient materials property prediction, interfacing modeling with experimental characterization, extracting data from scientific literature, and autonomous experimental and simulation campaigns. Chan holds leadership positions at major DOE projects including the Energy Storage Research Alliance (ESRA), and Midwest Integrated Center for Computational Materials (MICCoM) and chaired the 2024 DOE Basic Energy Science Roundtable on AI for Chemistry and Materials, is an associate editor at the ACS Journal Chemistry of Materials, a member of the Condensed Matter and Materials Research Committee of the National Academies of Sciences, and serves on the advisory boards for journals and NSF/DOE projects. Chan was elected a Fellow of the American Physical Society in 2024. Chan earned a PhD in Physics from the Massachusetts Institute of Technology.

Miguel A. Bessa

Member

MIGUEL A. BESSA is an Associate Professor of Engineering at Brown University, pioneering the field of data-driven computational mechanics. Bessa's research at the intersection of Computational Mechanics, Machine Learning, and Optimization is ushering in a new era of material and structural design using artificial intelligence. Instead of traditional trial-and-error, Bessa's group develops new computational methods that accelerate engineering discovery, with two recent examples being the creation of a supercompressible metamaterial using scalable Bayesian machine learning and the inverse design of a lightsail for interstellar space travel via neural topology optimization. A former Fulbright Scholar and Veni award recipient, Bessa quickly advanced from a Caltech postdoctoral position (2017) to an Assistant and then Associate Professor role at Delft University of Technology (2021) before joining Brown in 2022. Bessa earned his PhD in Mechanical Engineering from Northwestern University.

Keith Andrew Brown

Member

KEITH ANDREW BROWN is an Associate Professor of Mechanical Engineering, Physics, and Materials Science & Engineering, at Boston University. Brown runs an experimental research group that studies polymers with a major focus on accelerating materials research using self-driving labs, transformative formats for experiments, and machine learning. Brown has been a leader in the AI-accelerated materials research community and currently chairs the AI for materials development staging group of the Materials Research Society in addition to service to the Acceleration Consortium. Brown has co-authored over 90 peer-reviewed publications, six issued patents, and his work has been recognized through awards including the Frontiers of Materials Award from The Minerals, Metals, & Materials Society (TMS), being recognized as a "Future Star of the AVS," the Omar Farha Award for Research Leadership from Northwestern University, and the AVS Nanometer-Scale Science and Technology Division Postdoctoral Award. Prior to Boston University, Brown was a postdoctoral fellow at the International Institute for Nanotechnology with Chad A. Mirkin at Northwestern University. Brown earned an SB in Physics from MIT and a PhD in Applied Physics at Harvard University with Robert M. Westervelt.

Julia R. Greer

Member

JULIA GREER (NAS) is a Professor of Materials Science, Mechanics, and Medical Engineering at the California Technical Institute. Prior to starting the appointment as a faculty member at Caltech in June of 2007, Greer was a post-doctoral fellow at PARC, Palo Alto Research Center, from August of 2005 until May of 2007. Greer also worked on investigating the behavior of organic semiconductor - thin film transistors (OTFTs) as well as nano-ink-derived metals for jet-printing in flexible electronics. Greer's research group at Caltech works on multi-functional materials and devices, material synthesis, mechanics of hierarchical architectures, energy storage, additive nano-manufacture, and the mechanics and physics of nanomaterials. Greer has numerous awards, including the Kavli Early Career Award (MRS, 2014), ACS Nano Letters Young Investigator Award and Lectureship (2013), the Materials, Metals, and Minerals Society (TMS) Early Career Faculty Award (2013), the Society of Engineering Science (SES) Young Investigator Award (2013), Popular Mechanics Breakthrough Award (2012), and many others. Greer earned a BS in Chemical Engineering from Massachusetts Institute of Technology, and an MS and PhD in Materials Science and Engineering from Stanford University.

Linda Hung

Member

LINDA HUNG is a Senior Manager in the Energy and Materials Division at Toyota Research Institute (TRI), as part of the leadership team for its program in Accelerated Materials Design and Discovery. The group's research focuses on energy materials, integrating AI, data-driven methods, and automation to enhance human expertise and accelerate physical experiments. Linda's research background in computational materials science also includes density functional theory, theoretical spectroscopy, and high-performance computing. Linda serves on the editorial board of Digital Discovery since its launch in 2021 and the Scientific Advisory Committee of the Advanced Photon Source since 2024. Prior to Toyota, Linda held research positions at the École Polytechnique (France), the University of Illinois Chicago, and the National Institute of Standards and Technology. Linda earned a PhD in Applied and Computational Mathematics from Princeton University.

Suhas Mahesh

Member

SUHAS MAHESH is a Program Scientist in the AI Institute at Eric Schmidt's Schmidt Sciences, leading the AI for Science programs. Mahesh's primary expertise lies at the intersection of materials science and artificial intelligence, specializing in the use of "self-driving labs" to accelerate materials discovery. Mahesh's research has encompassed a range of systems, including photovoltaics, sensors, LEDs, and catalysts, and has led to collaborations with companies such as Google, Meta, Sony, and LG. Mahesh is a recipient of the Rhodes Scholarship, the Schmidt Science Fellowship, and an Acceleration Consortium Fellowship, among numerous best paper awards. Mahesh earned a PhD in physics from the University of Oxford and was recognized with a university thesis award.