



Materials in Extreme Environments: New Monitoring Tools and Data-Driven Approaches

Presented by the National Academies' Condensed Matter and Materials Research Committee
Under the auspices of the Board on Physics and Astronomy

October 5-6, 2022

Keck Center of the National Academies
500 Fifth Street, NW, Washington, DC 20001

Live-streaming via Zoom: Meeting ID sent upon registration

Registration web site: [Click here](#)

Day 1: October 5, 2022	
9:30 AM ET/ 6:30 AM PT	<p>Welcome and Introductions:</p> <p>Olivia A. Graeve Jacobs Faculty Scholar and Professor Department of Mechanical and Aerospace Engineering Director, Materials Science and Engineering Program Director, CaliBaja Center for Resilient Materials and Systems University of California San Diego</p>
<p>Morning Session Chair:</p> <p>Stefano Curtarolo Edmund T. Pratt Jr. School Distinguished Professor Department of Mechanical Engineering and Materials Science Duke University</p>	
9:40 AM ET/ 6:40 AM PT	<p>Jakoah Brgoch Associate Professor Department of Chemistry University of Houston</p> <p><i>Finding thermally robust superhard materials with machine learning</i></p>

10:20 AM ET/ 7:20 AM PT	Wendy Mao Professor Department of Geological Sciences SLAC Photon Science Directorate Department of Geophysics Stanford University <i>New materials at high pressure</i>
11:00 AM ET/ 8:00 AM PT	Nir Goldman Deputy Group Leader, Non-equilibrium Theory Lawrence Livermore National Laboratory <i>Machine learning tools for predictive simulations of materials under reactive conditions</i>
11:40 AM ET/ 8:40 AM PT	Eric Homer Associate Professor Department of Mechanical Engineering Brigham Young University <i>A high-throughput approach to obtain structure-property relationships: application to grain boundary structure and mobility</i>
12:20 PM ET	Lunch
Afternoon Session Chair: Horacio Espinosa James and Nancy Farley Professor of Manufacturing and Entrepreneurship Professor of Mechanical Engineering, Civil and Environmental Engineering Professor of Biomedical Engineering Director, Theoretical and Applied Mechanics Program, McCormick School of Engineering Northwestern University	
1:10 PM ET/ 10:10 AM PT	Christopher Weinberger Associate Professor Department of Mechanical Engineering Colorado State University <i>Ultra-high temperature ceramic phases and compositional complexity</i>
1:50 PM ET/ 10:50 AM PT	Penghui Cao Assistant Professor Department of Mechanical and Aerospace Engineering University of California, Irvine <i>Fundamental mechanisms under extreme environments and the role of machine learning</i>

2:30 PM ET	Break
2:50 PM ET/ 11:50 AM PT	<p>Shyue Ping Ong Professor Department of Nanoengineering University of California San Diego</p> <p><i>Designing extreme materials at scale with machine learning</i></p>
3:30 PM ET/ 12:30 PM PT	<p>Day 1 Panel</p> <p>Moderator:</p> <p>Joseph Poon William Barton Rogers Professor of Physics Department of Materials Science and Engineering University of Virginia</p> <p>Panelists:</p> <p>Aaron Stebner Associate Professor School of Materials Science and Engineering Georgia Institute of Technology</p> <p><i>Benchmarking machine learning modeling approaches to materials and manufacturing research and development</i></p> <p>Douglas E. Wolfe Professor Department of Materials Science and Engineering Pennsylvania State University</p> <p><i>Advanced materials and manufacturing techniques for radiation, thermomechanical, and thermochemical applications</i></p> <p>Elizabeth J. Opila Rolls Royce Commonwealth Professor of Engineering Department of Materials Science and Engineering University of Virginia</p> <p><i>Thermochemical stability of materials in extreme environments: probing fundamental aspects of degradation mechanisms</i></p>
5:00 PM ET/ 2:00 PM PT	<p>Day 1 Recap</p> <p>Alisdair Davey DKIST Data Center Scientist National Solar Observatory</p>
5:10 PM ET	Workshop Adjourned for Day 1

Day 2: October 6, 2022	
9:30 AM ET/ 6:30 AM PT	<p>Welcome and Introductions:</p> <p>Saryu Fensin Staff Scientist Materials Science in Radiation and Dynamics Extremes (MST-8) Los Alamos National Laboratory</p>
<p>Morning Session Chair:</p> <p>Thomas A. Witten Homer J. Livingston Professor Emeritus Department of Physics The University of Chicago</p>	
9:40 AM ET/ 6:40 AM PT	<p>Gregory B. Thompson University Distinguished Research Professor Department of Metallurgical and Materials Engineering The University of Alabama</p> <p><i>Thermo-mechanical testing and characterization in extreme environments</i></p>
10:20 AM ET/ 7:20 PM PT	<p>Elizabeth Rasmussen National Research Council Postdoctoral Fellow Thermophysical Properties of Fluids Group National Institute of Standards and Technology</p> <p><i>Status and gaps in thermodynamic metrology of materials in extreme environments</i></p>
11:00 AM ET 8:00 AM PT	<p>Dana D. Dlott William H. and Janet G. Lycan Research Professor of Chemistry Department of Chemistry University of Illinois Urbana-Champaign</p> <p><i>Tabletop hypervelocity launcher and optical pyrometry for high-throughput studies of extreme states of molecules in condensed phases</i></p>
11:40 AM ET/ 8:40 AM PT	<p>Aeriel D.M. Leonard Assistant Professor Department of Materials Science and Engineering The Ohio State University</p> <p><i>Advanced microscopy techniques for understanding dislocation interactions and damage in complex microstructures</i></p>
12:20 PM ET	Lunch

Afternoon Session Chair:

Raymundo Arroyave

Professor

Department of Materials Science and Engineering

Texas A&M University

**1:10 PM ET/
10:10 AM PT**

Maria K. Chan

Scientist

Center for Nanoscale Materials

Argonne National Laboratory

Where are the atoms? Towards real time inversion of characterization data

**1:50 PM ET/
10:50 AM PT**

Scott T. Misure

Inamori Professor

Kazuo Inamori School of Engineering

Alfred University

Reaction dynamics studied over large length scales using integrated in situ X-ray diffraction, Raman scattering and scanning electron microscopy

2:30 PM ET

Break

**2:50 PM ET/
11:50 AM PT**

Joshua C. Agar

Assistant Professor

Department of Mechanical Engineering and Mechanics

Drexel University

Codesign of parsimonious machine learning for high velocity materials microscopy on the edge

<p>3:30 PM ET/ 12:30 PM PT</p>	<p>Day 2 Panel</p> <p>Moderator:</p> <p>Duane D. Johnson Anson Marston Distinguished Professor of Engineering Department of Materials Science and Engineering Faculty Scientist, Ames Laboratory Iowa State University</p> <p>Panelists:</p> <p>Mathew J. Cherukara Group Leader, Computational X-ray Science Advanced Photon Source Argonne National Laboratory <i>HPC+AI-enabled X-ray science</i></p> <p>Jessica A. Krogstad Associate Professor Department of Materials Science and Engineering University of Illinois Urbana-Champaign <i>Indirectly tracking point defect accumulation and transport in ceramics through in situ ion irradiation and image analysis</i></p> <p>Blas P. Uberuaga Scientist Materials Science and Technology Division Los Alamos National Laboratory <i>Novel capabilities for studying irradiated materials</i></p>
<p>5:00 PM ET/ 2:00 PM PT</p>	<p>Final Remarks and Recap of the Workshop</p> <p>Andrew Minor Professor Department of Materials Science and Engineering Facility Director, National Center for Electron Microscopy Lawrence Berkeley National Laboratory University of California, Berkeley</p>
<p>5:15 PM ET</p>	<p>Workshop Adjourned for Day 2</p>