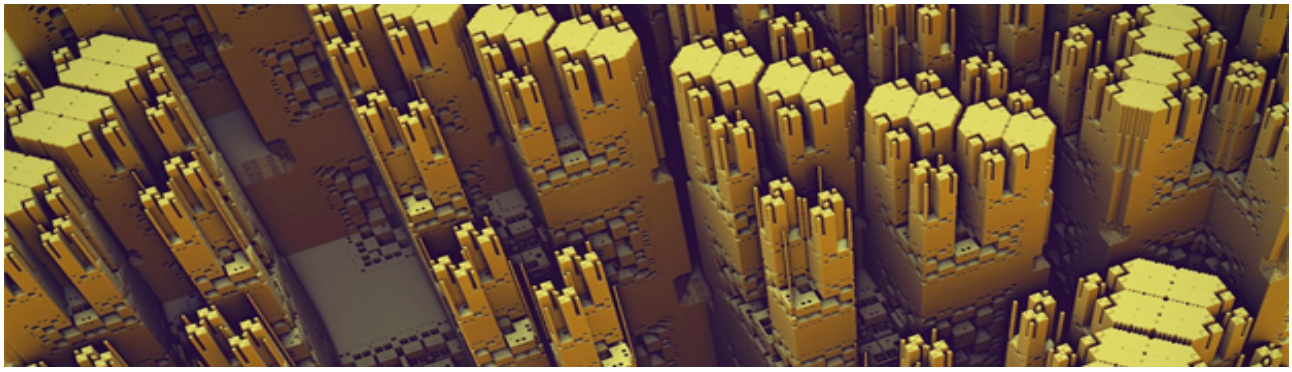
NATIONAL ACADEMIES Sciences Engineering Medicine

Autonomous Materials Discovery and Optimization



A DMMI Workshop

Keck Center, Room 206

500 Fifth Street, N.W.

Washington DC 2000

Presented by the National Academies' Defense Materials, Manufacturing and its Infrastructure Standing Committee (DMMI)

Chair DMMI - **Haydn Wadley**, UVA;
Workshop Chair - **Andrea Maria Hodge**, University of Southern California
Workshop Vice Chair - **Thomas Kurfess**, Georgia Institute of Technology

Under the auspices of the National Materials and Manufacturing Board (NMMB)

Autonomous materials are becoming a larger part of everyday life and manufacturing. This includes the advances in data analytics, AI, computational materials science, thermodynamic property prediction/data bases and autonomously operated synthesis, testing, and characterization techniques that are soon likely to reach, a point where the autonomous design of a material is feasible. Join the National Academies for a hybrid workshop on **November 1-2, 2022** to discuss global developments in the application of autonomy to materials science and manufacturing; unsolved challenges for autonomous material property prediction; and emerging needs for robotic tools for accelerated materials synthesis, characterization and testing. Some international speakers are remote.

Register to attend at http://dmmi.eventbrite.com

Workshop Agenda

Day 1: November 1, 2022	
10:00 am ET/ 7:00 am PT	**Welcome and Introduction**
10:10 am ET/ 7:10 am PT	**Overview and Topic Introduction:** Adam Rawlett, Army Research Laboratory
10:20 am ET/ 7:20 am PT	**Keynote:** Alan Aspuru-Guzik, University of Toronto **Discussion**
Session 1 Topic: Autonomous Materials Design *Topic leaders: Susan Sinnott and Klavs Jensen*	
11:00 am ET/ 8:00 am PT	**Speaker:** Ryan Dehoff, Oak Ridge National Laboratory
11:30 am ET/ 8:30 am PT	**Speaker:** Christoph Brabec, FAU Erlangen-Nürnberg
12:00 pm ET/ 9:00 am PT	**LUNCH BREAK**
1:00 pm ET/ 10:00 am PT	**Topic 1 Discussion:** Moderated by: Susan Sinnott Panelists: - Cosima Boswell-Koller, National Science Foundation - Adama Tandia, Corning Incorpoated - Francesca Tavazza, National Institute of Standards and Technology **Q+A and General Discussion**

Session 2 Topic: Testable Hypothesis Approaches *Topic leaders: Kelly Nygren and Ned Thomas*	
2:30 pm ET/ 11:30 am PT	**Speaker:** Rafael Gomez-Bombarelli, Massachusetts Institute of Technology
3:00 pm ET/ 12:00 pm PT	**Speaker:** Jason Hattrick-Simpers, University of Toronto
3:30 pm ET/ 12:30 pm PT	**BREAK**

Session 2 Topic: Testable Hypothesis Approaches *Topic leaders: Kelly Nygren and Ned Thomas*	
3:45 pm ET/ 12:45 pm PT	**Topic 2 Discussion:** Moderated by: Kelly Nygren Panelists: - Benji Maruyama - Air Force Research Laboratory - Andy Detor - Defense Advanced Research Projects Agency - Horst Hahn - KIT & University of Oklahoma **Q+A and General Discussion**
5:15 pm ET/ 2:15 pm PT	**Recap of the Day**
5:30 pm ET/ 2:30 pm PT	**Adjourn for the day**

Day 2: November 2, 2022	
10:00 am ET/ 7:00 am PT	**Welcome, DMMI Introduction, and Day 2 Introduction**
10:15 am ET// 7:15 am PT	**Keynote:** Jed Pitera, IBM Almaden Research Center **Discussion**
Session 3 Topic: Autonomous Characterization and Property Measurement Tools *Topic leaders: Robert Hull and David Aspnes*	
11:00 am ET// 8:00 am PT	**Speaker:** Anna Lena Eberle, Carl Zeiss MultiSEM GmbH
11:30 am ET// 8:30 am PT	**Speaker:** Nazanin Bassiri-Gharb - Georgia Institue of Technology & National Science Foundation
12:00 pm ET// 9:00 am PT	**LUNCH BREAK**

1:00 pm ET/ 10:00 am PT	**Topic 3 Discussion:** Moderated by: **Robert Hull** Panelists: - Ken Vecchio, University of California San Diego - Brad Boyce, Sandia National Laboratories - Brian Sheldon, Brown University - Tonio Buonassisi - Massachusetts Institute of Technology **Q+A and General Discussion**

Session 4 Topic: Smart Process Tools *Topic leaders : John Koszewnik, Lourdes Salamanca-Riba*	
2:30 pm ET/ 11:30 am PT	**Speaker:** Satyandra K. Gupta, University of Southern California
3:00 pm ET/ 12:00 pm PT	**Speaker:** Satish Bukkapatnam, Texas A&M University
3:30 pm ET/ 12:30 pm PT	**BREAK**
3:45 pm ET/ 12:45 pm PT	**Topic 4 Discussion:** Moderated by: **Lourdes Salamanca-Riba** Panelists: - Gilad Kusne, National Institute of Standards and Technology - Prasana Balachandran, The University of Virginia - Michael Thompson, Cornell University **Q+A and General Discussion**
5:15 pm ET/ 2:15 pm PT	**Recap of the Workshop**
5:20 pm ET/ 2:20 pm PT	**Discussion of future study topics**
6:00 pm ET/ 3:00 pm PT	**Adjourn Workshop**