

Frontiers of AI-Realized Metastable Materials May 8, 2026

1:20	<u>Session 3: AI-guided predictions of metastable materials</u> <i>(25 minute presentations each, all questions saved for moderated panel at session end)</i> <i>Moderator: Archana Raja, Staff Scientist, Lawrence Berkeley National Laboratory</i>	
1:20-1:45	Learning thermodynamic landscape & kinetic pathways in materials synthesis	Subramanian (Subbu) Sankaranarayanan <i>Professor, University of Illinois Chicago</i>
1:45-2:10	[Automation for materials discovery and synthesis]	Peter Beaucage <i>Senior Director, Lila Sciences</i>
2:10-2:35	Evaluating the synthesizability of predicted metastable materials beyond the DFT convex hull	Wenhao Sun <i>Assistant Professor, University of Michigan</i>
2:35-3:05	Moderated Q&A and Discussion Panel	
3:05	<i>Break (30 minutes)</i>	
3:35	<u>Session 4: Breakout discussions</u>	
3:35-3:45	Breakout Guidance and Discussion Prompts: <i>(10 minutes)</i>	Maria Chan and Raymundo Arroyave <i>Workshop Co-chairs</i>
	<ul style="list-style-type: none">- What are some of the ideas discussed today that resonated with you and would be exciting directions to pursue? Based on your own expertise, are there additional directions or synergies that should be explored?- What are some metastable materials systems that are of interest to you? How do you think AI tools will be able to assist in the development of such?- What AI tools are you involved in or interested in which may be brought to bear in the development of metastable materials? If you can have an AI tool "wish list", what would be on it?- What are some current bottle necks you are dealing with, or you can envision, for the experimental realization of metastable materials? How might AI and automation assist in overcoming these challenges?	
3:45-4:45	Breakout groups <i>(60 minutes)</i>	All in-person attendees
4:45-5:15	Breakout Summaries <i>(3 groups, 10 minutes each)</i>	All attendees
5:15-5:35	Moderated Q&A and Discussion Panel	All attendees
5:35	Closeout <i>(10 minutes)</i>	Maria Chan and Raymundo Arroyave <i>Workshop Co-chairs</i>
5:45	<i>Adjourn workshop</i>	

IMPORTANT NOTES

Presenters:

- Please do not include ITAR-controlled or sensitive information in your presentation.
- A National Academies Board staff member will ask you to sign a form before the meeting allowing us permission to use your likeness and presentation for our livestream video, which will be posted on our Board website after the meeting. Please get in touch with us before the meeting if you have any concerns about this usage.

(agenda information continues on page 3)

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Committee & Board Members and Presenters:

- Remote access will be provided through Zoom. This will allow you to participate in the meeting even if you can't be physically present.
- Please note that Zoom allows audio and any materials exchanged or viewed during the session to be recorded and shared.
- By participating in this activity, you agree to let your voice, likeness, and any materials you provide be recorded for use and dissemination. This includes any language, format, or media now known or later devised.
- You release the National Academies of Sciences, Engineering, and Medicine from any and all claims, liability, or damages arising from any such use. If you disagree, please do not join the session.

THANK YOU ALL FOR YOUR COOPERATION, AND WE LOOK FORWARD TO A SUCCESSFUL MEETING.