

**Symposium on “AI for Materials: From Discovery to Production”  
October 6-7, 2020**

**DAY 1: Tuesday, October 6, 2020 | 10:30 AM – 5:30 PM**

**10:30 am**                      **Opening Remarks:** The New York Academy of Sciences

*Physics and Causality in Machine Learning*

*Session Leads: Payel Das, Sergei V. Kalinin*

*Developing methodologies to unravel physics laws and causality from machine learning predictions, to avoid using AI as a black box in materials science. Efforts of integrating experimental and computational data into the same databases will also be discussed.*

**10:35 am**                      **Keynote Address #1: Leon Bottou, Facebook**

**11:10 am**                      Presentation Session #1: Carla Gomes, Cornell; Rama Vasudevan, ORNL

**12:00 pm**                      **Short Break**

**12:10 pm**                      Presentation Session #2: Alexandra Boltasseva, Purdue University; Two other speakers from presentation abstract submissions

**1:20 pm**                      **Break and Virtual Poster Session**

*Data Infrastructures*

*Session Leads: Anatoly Frenkel, Kristin Persson*

*Improving the existing data infrastructures used in materials science research to facilitate easier integration and transfer of data for the application of AI, and to promote a better data sharing environment in the field.*

**2:20 pm**                      **Keynote Address: Rampi Ramprasad, PhD, Georgia Tech**

**2:55 pm**                      Presentation Session #3: Matthias Scheffler, FHI Berlin; Jason Hattrick-Simpers, NIST

**3:45 pm**                      **Short Break**

**3:55 pm**                      STAR\* Talks: Speakers TBD from poster abstract submissions\*

**4:15 pm**                      Presentation Session #4: Tonio Buonassisi, MIT; Two other speakers from presentation abstract submissions

**5:25 pm**                      **Day 1 Wrap Up/Day 2 Preview**

**5:30 pm**                      **Close of Day 1**

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\* (STAR = Short, Topical, Accomplished, Relevant) A series of short early career investigator presentations across a variety of topics at the frontiers of AI for materials science. Selected from Poster Abstract submissions.

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**DAY 2: Wednesday, October 7, 2020 | 9:00 AM – 1:30 PM**

**9:00 am**            **Opening Remarks:** Event Sponsor/The New York Academy of Sciences

*AI in Materials Production and Industry*

*Session Leads: Mat Halls, Josh Schrier*

*Promoting the application of AI to address industry-related issues in materials science, including the scalability of materials production from the lab to the factory, the synthetic and catalytic routes of new materials, and the application of AI to achieve “closed loop” production pathways.*

<b>9:05 am</b>	<b>Keynote Address: Nobuyuki N. Matsuzawa, Panasonic Corporation</b>
<b>9:40 am</b>	Presentation Session #5: Michael Helander, OTI Lumionics; Elsa Olivetti, MIT
<b>10:30 am</b>	<b>Break and Virtual Poster Session</b>
<b>11:00 am</b>	Panel Discussion: Closed loop production through AI: Automating the design, build, test, and learn cycle
<b>11:50 am</b>	Presentation Session #6: Muratahan Aykol, Toyota Research Institute, Toronto; Two other speakers from presentation abstract submissions
<b>1:00 pm</b>	Session Summaries: 8 minutes each (Session Chairs)
<b>1:25 pm</b>	<b>Final Remarks:</b> The New York Academy of Sciences
<b>1:30 pm</b>	<b>End of Day 2</b>