September 25–26, 2018
Embassy Suites by Hilton Pittsburgh Downtown • Pittsburgh, PA

Course Agenda

Current as of September 20, 2018.

Time	Description
Tuesday, September 25	
8:00 a.m. to 8:30 a.m.	Welcome and Course Overview (J. Tappan, Citrine Informatics, and TMS)
8:30 a.m. to 9:30 a.m.	**KEYNOTE**: Motivation for Applying ML to Materials (B. Meredig, Citrine)
9:30 a.m. to 10:00 a.m.	Coffee & Networking Break
10:00 a.m. to 11:00 a.m.	Machine Learning 101 (E. Antono, Citrine) *Introduction to machine learning in materials science*
11:00 a.m. to Noon	Decoding the Glass Genome (J. Mauro, Pennsylvania State University) *Glasses have played a critical role in the development of modern civilization and will continue to bring new solutions to global challenges from energy and the environment to healthcare and information/communication technology. To meet the accelerated pace of modern technology delivery, a more sophisticated approach to the design of advanced glass chemistries must be developed to enable faster, cheaper, and better research and development of new glass compositions for future applications. In the spirit of the U.S. Materials Genome Initiative, here we describe an approach for designing new glasses based on a mathematical optimization of composition-dependent glass property models.*
Noon to 1:00 p.m.	Lunch (provided)
1:00 p.m. to 2:00 p.m.	Demystifying Machine Learning Algorithms (E. Antono, Citrine) *In this talk, Erin Antono will give an overview and comparison of some of the most common machine learning algorithms and their applications to materials research and development.*
2:00 p.m. to 2:15 p.m.	Coffee & Networking Break
2:15 p.m. to 3:30 p.m.	Sequential Learning Workshop – Building a Machine Learning Model from Materials Data (J. Tappan, Citrine) *Attendees will participate in a hands-on workshop demonstrating the workflow and analysis involved in sequential learning.*
3:30 p.m. to 3:40 p.m.	Coffee & Networking Break
3:40 p.m. to 5:00 p.m.	Sequential Learning Workshop Part 2 – Model Iteration and Analysis (J. Tappan, Citrine)

5:30 p.m. to 7:30 p.m.	Happy Hour at Sienna Mercato – Il Tetto Rooftop 942 Penn Avenue, Pittsburgh, PA 15222 *We will walk to Il Tetto from the Embassy Suites after the course ends for the day. The walk is approximately 5 minutes. Complimentary drinks and hors d'oeuvres will be provided.*
Wednesday, September 26	
8:30 a.m. to 9:30 a.m.	Case Discussion – Application of Materials Informatics (B. Meredig, Citrine) *Bryce Meredig will lead a case discussion about different industrial and academic applications of machine learning in materials science.*
9:30 a.m. to 10:30 a.m.	Applying Machine Learning to Materials Discovery (C. Wolverton, Northwestern University)
10:30 a.m. to 11:00 a.m.	Coffee & Networking Break
11:00 a.m. to Noon	The MGI & Data-driven High-Throughput Synthesis and Characterization (J. Hattrick-Simpers, NIST) *Jason Hattrick-Simpers will discuss NIST's role in the Materials Genome Initiative, their recent work in data-driven high-throughput synthesis, and characterization, the emerging High-Throughput Experimental Materials Collaboratory, and the impact these efforts can have on the materials industry.*
Noon to 1:00 p.m.	Lunch (provided)
1:00 p.m. to 2:00 p.m.	Neural Networks and Their Application to Materials Research and Development (B. DeCost, NIST)
1:00 p.m. to 3:00 p.m.	Data Workshop (Citrine) *Participants will learn how to:* *1. Structure materials data for machine learning and data analysis* *2. Apply data analysis tools to materials datasets* **Citrine will provide data for participants who cannot bring their own*
3:00 p.m.	Course Concludes