



# Emerson Center Lectureship Award Symposium

## Advancing Molecular Sciences by Machine Learning and Quantum Computing

October 11, 2019,  
Oxford Road Building Presentation Room

**AWARD WINNER &  
KEYNOTE SPEAKER**

**Prof. Alan Aspuru-Guzik,**  
University of Toronto, Canada

### The Materials for Tomorrow, Today



In this talk, I argue that for materials discovery, one needs to go beyond simple computational screening approaches followed by traditional experimentation. We have been working on the design and implementation of what we call “materials acceleration platforms” (MAPs). MAPs are enabled by the confluence of three disparate fields, namely artificial intelligence (AI), high-throughput quantum chemistry (HTQC), and robotics. The integration of prediction, synthesis and characterization in an AI-driven closed-loop approach promises the acceleration of materials discovery by a factor of 10, or even a 100. I will describe our efforts under the Mission Innovation umbrella platform around this topic.

#### INVITED SPEAKERS

#### EVENTS SCHEDULE



**Francesco Evangelista**  
Department of  
Chemistry,  
Emory University

2:15 – 2:45

#### OPENING CEREMONY & AWARD PRESENTATION

2:45 – 3:45

**Alan Aspuru-Guzik:** **The Materials for Tomorrow, Today**

3:45 – 4:35

**Francesco Evangelista:** **Electronic Structure Challenges for Quantum Computing**



**Matthew S. Sigman**  
Department of  
Chemistry,  
The University  
of Utah

4:35 – 4:50

#### COFFEE BREAK

4:50 – 5:40

**Matthew Sigman:** **Developing Modern Data Analysis Tools for Synthesis & Catalysis**

5:40 – 6:30

**Rampi Ramprasad:** **Polymer Genome: A Machine Learning Platform for Rational Polymer Design**



**Rampi Ramprasad**  
School of Materials  
Science and  
Engineering,  
Georgia Institute of  
Technology,

6:30 – 6:40

#### CLOSING

6:40 – 9:00

**DINNER (by invitation)**

**Co-  
SPONSORS:  
REGISTRATION:  
CONTACT:**



**DEPARTMENT OF CHEMISTRY**

**THE HIGHTOWER FOUNDATION;**

<http://www.emerson.emory.edu/conferences/form/register.html>

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**Registration is free.**