The Materials for Tomorrow, Today

Alan Aspuru-Guzik[a]

[a] *University of Toronto, 80 St. George St., Toronto, Ontario, M5S 3H6, Canada*
alan@aspuru.com

In this talk, I argue that for materials discovery, one needs to go beyond simple computational screening approaches followed by traditional experimentation. I have been working on the design and implementation of what I 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.