Autonomous laboratory: Self-driving labs to accelerate battery cathode material discovery

Dylan Perry, Derek Li, Prachi Shah, Barry Zhang, Zoya Sadighi, Sarish Rehman, Keli Chiu, Luis Martin Mejia Mendoza, Shayan Mousavi Masouleh, Scott R. Smith
National Research Council (NRC) Canada, Clean Energy Innovation Research Center
2620 Speakman Dr, Mississauga ON, Canada
Scott.Smith@nrc-cnrc.gc.ca

Canada's target for net-zero greenhouse gas emissions by 2050 necessitates increased electrification. The Canadian Critical Mineral Strategy seeks to enhance the supply chain for battery materials by addressing processing challenges with battery and electric vehicle (EV) manufacturing. Despite Canada's mineral exploration projects, significant production and processing of lithium battery materials are hindered by economic, market, and supply chain limitations. The Critical Battery Materials Initiative (CBMI), a $40 million NRC initiative, utilizes innovative acceleration platforms that can leverage automation coupled with AI/ML frameworks for; 1) materials discovery of novel cathode materials for energy storage applications, as well as 2) process optimization of extracting and recovery of critical battery minerals from primary and secondary feedstocks. Therefore two acceleration platforms that utilize self-driving lab and artificial intelligence approaches to develop more efficient and sustainable pathways and discover new sustainable battery materials are being developed. These projects seek to advance battery materials discovery, process control, and data acquisition for battery material production in Canada at the newly opened Terra-Canada Mississauga facility, which is the National Research Council of Canada's Centre of Excellence in accelerated material discovery and process optimization.

Here, we will introduce our custom and modular acceleration platforms and provide progress updates on; 1) our efforts to automate our acceleration platforms to accelerate time required to conduct research investigations, and 2) utilizing AI for guided discovery and optization campaigns with the goal of intelligently reducing the number of experiments to reach a target. This work strives to demonstrate how AI, machine learning, and laboratory automation can improve the pace at which research and development can be conducted as well as how new capabilities can be achieved with automated and AI process controls.