Integration of AI and robotics with materials sciences will lead to new clean energy technology

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Materials are the foundation of essentially all clean energy technologies including advanced batteries, solar cells, low-energy semiconductors, catalysts for capturing and storing CO2, and more. But discovering new materials is currently a time consuming and expensive process: to determine whether they will be useful, newly discovered molecules are run through simulation, synthesis, and testing in an expensive process that can take 10 to 20 years.

Artificial intelligence and robotics combined with material sciences and other advanced methods could dramatically speed up development of new materials for all clean-energy technologies. The proposed integrated Materials Acceleration Platforms (MAPs) could cut the average time for developing a useful new material from 20 years down to one or two years.

The Expert Workshop Report, "Materials Acceleration Platform: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence," was released in Mexico City today. This work is the result of a September 2017 workshop that convened more than 55 leading scientists from around the world to define the challenges, opportunities, and fundamental research needs related to materials discovery. The workshop was sponsored by the Mexican Ministry of Energy (SENER), the U.S. Department of Energy, and CIFAR.

This Report is an important milestone of the Clean Energy Materials Innovation Challenge of the global initiative Mission Innovation (MI) of 22 countries and the European Union that aims to accelerate global clean energy innovation. The Report calls for integrating material sciences with next-generation computing (high-throughput), artificial intelligence (machine learning) and robotics to accelerate the pace of materials discovery. Among the recommendations are development of "self-driving/autonomous laboratories" that automatically design, perform and interpret experiments in the quest of new high-performance, low-cost materials.

"The performance, efficiency and affordability of clean energy technologies can be increased by finding materials with the properties you need. At the moment, we're very much like Edison looking for filaments for his light bulb, testing them one by one in a sequential fashion, by trial-and-error, until we find the one that works. This report lays out a road map for methods that will let us quickly discover and design materials with exactly the properties we need. The key is to create fully integrated MAPs from beginning to end that enable humans to accelerate their pace of discovery," said Alán Aspuru-Guzik from Harvard University, co-chair of the workshop and lead author of the report.

The panel's recommendations

The workshop makes six recommendations that will lead to what it calls materials acceleration platforms (MAPs) that would integrate automated robotic machinery with rapid synthesis and characterization of materials and artificial intelligence that would accelerate the pace of discovery.

The platforms would help researchers transition from a largely trial-and-error method of materials discovery to one of "inverse design," in which materials with desired properties could be easily searched for and

developed.

The workshop report recommends six key areas which will need to be developed to create these materials acceleration platforms. They are:

- 1) "Self-driving laboratories" that design, perform and interpret experiments in an automated way;

2) The development of specific forms of AI for materials discovery;

3) Modular materials robotics platforms that can be assemblies of modular building blocks for synthesis and characterization;

4) Further research into computational methods for inverse design;

5) New methodologies for bridging the length and timescales associated with materials simulation; and

6) Sophisticated data infrastructure and interchange platforms.

The report emphasized the need to develop multidisciplinary international teams of scientists and engineers with expertise in chemistry, materials sciences, advanced computing, robotics and AI, among other disciplines.

"I'm pleased that CIFAR was able to contribute to Mission Innovation's important work," said CIFAR President & CEO Alan Bernstein. "CIFAR and MI share similar goals, and our emphasis on excellence, global participation and tackling tough questions is the best strategy for creating the disruptive technologies needed to address the world's growing demand for energy."

Dr. Hermann Tribukait, of Mexico's Energy Innovation Funds and a

report co-author, stated that "The private-sector stakeholders that join this initiative early will presumably have a first-mover advantage, that is, they will cultivate the know-how to adjust and gain a larger share of the growing benefits from these new technologies."

More information: Copies of the report can be downloaded at: www.cifar.ca/wp-content/upload … ovationIC6Report.pdf

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