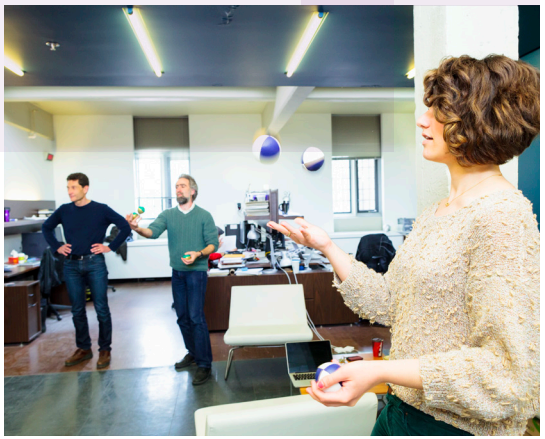
Research Impact: Machine learning accelerates development of materials to make sustainable batteries and increase aircraft fuel efficiency



The Computational Materials Engineering Laboratory (CMEL) at the University of Toronto is an outstanding example of how digital research infrastructure is facilitating advances in areas critical to humankind such as climate change. The CMEL team, led by Dr. Chandra Veer Singh, Associate Professor of Materials Science and Engineering, is developing efficient machine learning models to accelerate materials development, which has historically required a slow and cumbersome trial-and-error approach.

In machine learning, "data is everything," says Abu Anand, a PhD student on the team. In collaboration with other research groups, CMEL builds quality databases related to specific materials and alloys, then applies machine learning techniques to predict material properties. Eventually, the team intends to make the databases open source, available to researchers around the globe.

The CMEL team is focused on identifying properties that can be leveraged to improve energy sustainability in a variety of ways, such as making aircraft more fuel-efficient and batteries more long-lasting. Researchers in the lab work in several areas:

- Graphene and other two-dimensional materials
- Batteries and energy materials
- Alloy design
- 'Meta' materials (materials whose structure has been changed to reduce weight while retaining strength)

From left to right: Dr. Zhiwen Chen, Adwitiya Rao, Jonathan Shan, Prof. Chandra Veer Singh, Sahar Choukir, Eric Nicholson, Abu Anand, Dr. Shwetank Yadav, Farzin Najafi, Hema Rajesh Nadella, Pedro Guerra Demingos, Zhuole (Joller) Lu, Szu-Jia (Jessica) Liu, Dr. Lixin Chen, Xiang Ni.

Anand's research focuses on high-entropy alloys. This field has emerged relatively recently. High-entropy alloys, which can withstand extreme temperatures, are of high interest in the automotive and aerospace sectors. Once perfected, these alloys will be 'game-changers', Anand says. "This is like the development of steel 100 years ago. These are the materials of the future."

While some projects at CMEL are still in the data-building stage, others are beginning to produce results. Last October, for example, Singh, Zhuole Lu, and Dr. Zhiwen Chen published a paper in the journal *Matter* to share significant findings related to the use of high-entropy alloys as catalysts for reactions. Such reactions include splitting water atoms to release hydrogen, which enables the use of hydrogen as a clean fuel. Using alloys as catalysts can potentially speed up and fine-tune chemical reactions, but the same complex combination of properties that allows them to do so also makes them difficult to research without the assistance of machine learning and sophisticated data management.

Anand says that he alone generates 1.5 terabytes of data every couple of months — data which then must be skillfully boiled down to 100 gigabytes without losing any important information. That's where SciNet, the advanced computing centre led by University of Toronto, comes in. SciNet provides access to high-performance computing cycles and supports post-processing of data and secure file management with their expertise.