Project Title: Seven MEng projects about multiscale mechanics, materials design, additive manufacturing and applied machine learning.
Supervisor: Prof. Yu Zou (MSE & MIE)
Disciplines Required: ME, MSE, EE, ChemEng or CIV
Start Date: Any time
End Date: at least for a semester
Application documents: CV, transcripts, and a short summary of research experience (if available)
NDA: No

1. **Electro-plastic and Plasto-electricity (also photo-plasticity) Effects in Small-scaled Ionic Crystal Systems and Semiconductors**

Doped ionic crystals exhibit phenomena called electro-plasticity and plasto-electricity. Interacting with charged vacancies, dislocations can carry charge, interact with an external electric field and thus affect plasticity, or they cause an electric current upon plastic deformation. This research plan focuses on exploring these only poorly studied phenomena at small length scales, i.e. between several microns down to below 100 nanometers.
Please refer to this paper https://science.sciencemag.org/content/360/6390/772/tab-pdf

2. **Inverse design of biomedical implant materials via a high-throughput highway**

Human civilization has been pushed forward by the discovery of new materials. Over the past centuries, metallic materials have been the major workhorse of our society, thanks to their unique and irreplaceable properties. For example, metallic joint replacement is one of the most successful procedures in all of medicine. However, joint replacement may fail earlier than it is supposed to last – redoing replacements, or revision surgeries, are needed. The early failure of the joint implant, significantly reducing the function of patients and placing a heavier burden on the health care system (137 million annually in Canada). This failure is most associated with implant materials. The discovery of new metallic implant materials, however, has been a slow and arduous task, even nowadays. The urgent need in the health care system, however, poses a challenge to speed up the rate of screening materials for creating new implant materials with a combination of outstanding properties. Our collaborative research team includes expertise in materials science, computational science, mechanical engineering, surgery, and biomedical engineering.
References https://science.sciencemag.org/content/361/6400/360
https://www.nature.com/articles/s41467-019-09700-1

3. **Design and manufacture of novel wear-and-erosion resistant high-entropy alloys**

Equipment used in mineral, oil and gas industries often suffer from severe wear and erosion degradation during operation, such as pumps, valves, cones, impeller, crushers, and ground engagement tools. The wear or erosion induced early failure of these products significantly reduce the service of life of these machines, and, consequently, increase the product and service cost. The academic team at the University of Toronto will collaborate with the Weir Group Plc technical staff to design and fabricate new metallic materials that can significantly improve the wear-and-erosion resistant properties for the components of the mineral, oil and gas products. This project will be focused on an emerging alloy system – high-entropy alloys (HEAs). HEAs are loosely defined as solid-solution alloys that are made of five or more metallic elements in equimolar or near-equimolar ratios, wherein multiple principal elements show a strong tendency of solid-solution hardening effects but also exhibit superior toughness. The search for new HEAs with optimal mechanical properties will be based on a high-throughput combinatorial method.
References https://science.sciencemag.org/content/345/6201/1153
https://www.nature.com/articles/nature17981

4. Nanostructured high-entropy alloys as next-generation catalysts for energy applications: from AI-driven accelerated discovery to mass production

Metallic nanoparticles are of interest in a wide range of energy applications, including electrocatalysis, energy storage, and water splitting. Conventionally, such nanoparticles are limited by pure metals, binary or ternary alloys, generally containing noble metals (e.g., Ru, Pt, and Pd). The discovery of new low-cost, high-efficiency catalysts has been highly desirable for decades. High-entropy alloys (HEAs) – solid-solutions made of five or more metallic elements with *equimolar*/*near-equimolar* ratios – exhibit excellent mechanical properties (*1*-*3*). Very recently, a few studies have shown that some HEAs also show extraordinary functional properties, especially for catalysis (e.g., ammonia oxidation, hydrogen storage, electrocatalysis, oxygen reduction reaction, and water splitting. The machine learning approach can greatly speed up the discovery of new HEAs for energy applications. Integrated with high-throughput experimentation, the AI and robotics-enabled methodology will provide a new avenue for discovering new HEAs as next-generation catalysts. Towards industrial applications, mass production of HEA nanoparticles is necessary, requiring extreme fabrication conditions, such as ultrahigh heating/quenching rates. Thermal plasmas are capable of rapid heating and cooling of materials (9), thus well suited for large-scale synthesis of HEA nanoparticles.
Ref. Y. Yao *et al.*, Carbothermal shock synthesis of high-entropy-alloy nanoparticles. *Science* **359**, 1489-1494 (2018). https://science.sciencemag.org/content/359/6383/1489.abstract

P. Xie *et al.*, Highly efficient decomposition of ammonia using high-entropy alloy catalysts. **10**, 1-*Nature commnications* 12 (2019).

5. **Autonomous additive manufacturing system (AAMS): a novel in-situ monitoring and closed-loop control process using machine learning**

Metal additive manufacturing (M-AM), or metal 3D printing, is a process in which a laser fuses metallic powder to build up parts layer-by-layer directly from 3D digital models. Metal AM will fundamentally change the entire manufacturing industry, from aerospace to biomedical sectors, by 2025 (McKinsey Report, 2019). A key hurdle for the mass adoption of AM is the formation of flaws, such as pores, cracks and other defects, during the manufacturing process, leading to inconsistent product quality. To reduce defect density, it is essential to identify optimal processing parameters (laser power, spot size, scanning speed, and many more) for each material/geometry. However, the sheer size of the parameter space makes it a daunting task. Ideally, *adaptive* control of the parameters during manufacturing is highly desirable, especially for parts made of multi-materials and with complex geometries.

https://www.nature.com/articles/s41563-019-0408-2.pdf?origin=ppub
https://science.sciencemag.org/content/363/6429/849.abstract

6. **Data-driven topology and microstructure optimization in metal 3D printing**

Metal 3D printing, also known as metal additive manufacturing (AM), offers a unique opportunity for rapid fabrication of metallic components with complex macrostructure (topology) and microstructure (grain/phase size and orientation). Processing conditions (e.g., cooling rate and thermal gradient) influence both macrostructure and microstructure, and eventually, the final properties of products. Scientific challenges in metal 3D printing stem from the diverse processing conditions and their unknown effects on the evolution of various topological and microstructural features, leading to unpredictable performance of components.

Refs. https://www.nature.com/articles/s41586-019-1783-1
https://www.nature.com/articles/nature23894
https://www.nature.com/articles/s41586-018-0850-3

7. High-entropy alloys for Material Recycling

High-entropy alloys (HEAs) are a promising new materials class that may offer enhanced mechanical, electrical, magnetic, or electrochemical properties over conventional metals and alloys. HEAs are typically defined as alloys made up of 5 or more elements, each in the compositional range of 5-35 at%, that form a single solid-solution phase. Other terms such as medium-entropy alloys (MEAs), complex concentrated alloys (CCAs), and multi-principal element alloys (MPEAs) define various sub-classes of HEAs that may contain less than 5 elements, multiple phases, or non-metallic elements. While many of the HEAs investigated to date exhibit good mechanical properties in comparison to high-performance materials such as stainless steels and superalloys, the factor that severely limits their potential applications is that of cost. In conventional materials, the base element (e.g. Fe, Al) is often inexpensive in comparison to their alloying elements (Ni, Co, Mo, Cu). However, the near-equimolar range in composition of HEAs would drive the cost of these materials to unacceptable levels. The recycling industry in one area that we believe could offer some relief to the high cost of HEAs. To begin this study, there are 2 preliminary goals: (1) Identify the class(es) of recycled materials for which this would have the highest impact (cost, time, environment). (2) Identify the alloys within these classes which could be combined to form either (i) well-studied HEAs, or (ii) new compositions of HEAs.