DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Fall Seminar Series

Combinatorial Experimentation and Machine Learning for Materials Discovery

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Professor

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PISB 104

Throughout the history of humankind, scientists and engineers have relied on the slow and serendipitous trial-and-error approach for materials discovery. In the 1990s, the combinatorial approach was pioneered in the pharmaceutical industry to dramatically increase the rate at which new medical compounds are identified. The high-throughput concept is now widely implemented in a variety of fields in materials science. Dr. Takeuchi's group has developed combinatorial thin film synthesis and characterization techniques in order to perform a rapid survey of previously unexplored materials phase space in search of new inorganic functional materials with enhanced physical properties. Over the years, the challenges in the high-throughput approach has evolved from the synthesis of a large number of disparate compounds to the development of quantitatively accurate rapid characterization tools to the analysis and digestion of a large amount of data churned out by the methodology. To address the last challenge, Dr. Takeuchi's group is increasingly relying on machine learning techniques including pattern recognition within diffraction data to construct phase diagrams and mining experimental databases to look for trends in materials properties for future predictions. Dr. Takeuchi will also discuss his group's latest effort where active learning is used to design and steer the sequence of experiments to maximize attainable knowledge, minimize experimental resources and, as a result, to further speed up the materials discovery process.

Dr. Ichiro Takeuchi is a professor of materials science and engineering and affiliated professor of physics at the University of Maryland. Dr. Takeuchi obtained his Bachelor of Science in physics from the California Institute of Technology and his PhD in physics from the University of Maryland. Dr. Takeuchi is the Graduate Program Director in the Department of Materials Science and Engineering at Maryland. He was a postdoctoral researcher at Lawrence Berkeley National Laboratory, where he helped to pioneer the combinatorial materials discovery methodology. He previously also spent a number of years as technical staff at NEC Corporation, where he worked on thin film materials for superconducting electronics. Dr. Takeuchi is a Fellow of the American Physical Society. He won the University of Maryland Invention of the Year Award in 2010 for the invention of elastocaloric cooling. Dr. Takeuchi was awarded the University of Maryland Distinguished Scholar Teacher and the Outstanding Faculty Research Award in 2018.