

The 312th MANA Seminar



Data driven approaches to combinatorial discovery of functional materials Chair: Dr. Toyohiro Chikyow (MANA PI)

Prof. Ichiro Takeuchi

*(Department of Materials Science and Engineering,
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We are developing techniques to integrate theoretical materials designs and databases with combinatorial experimentation. Our research focus is on multifunctional and smart materials where enhanced physical properties are often associated with structural transitions. Current topics include search for rare-earth free permanent magnets, lead-free piezoelectrics, and new superconductors. Rapid x-ray diffraction screening plays a central role in all of our investigations. Directly incorporating database activities into combinatorial experimentation has always been a challenge in the community. We are developing techniques to quickly analyze experimentally obtained data together with entries from the Inorganic Crystal Structure Database (ICSD), which contains over 140000 entries. I will discuss our recent demonstration, where synchrotron diffraction data are analyzed live using machine learning techniques to decipher the structural phase distribution across ternary metallic composition spreads.

Venue: Auditorium, 1F, WPI - MANA Bldg.

Namiki site

Date: February 8th, Friday

Time: 15:30-16:15

Contact: International Center for Materials Nanoarchitectonics (MANA), Nakayo Nakata (ex. 8806)