

The 124th GREEN Seminar



Accelerating Materials Discovery: Combining AI, In-Situ XRD, and TTT Diagrams for Rational Synthesis

Chair: Dr. Marcela Calpa(GREEN)

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This talk will present our recent advances in rational inorganic synthesis, moving beyond traditional trial-and-error. One approach combines an AI-guided strategy with in-situ synchrotron X-ray diffraction, highlighting both the capabilities and limitations of large-scale computational prediction in materials discovery. To understand the synthesis pathways of metastable materials, we constructed high-time-resolution SXRD and computational nucleation-limited Time-Temperature-Transformation (TTT) diagrams for the Li_3PS_4 solid electrolyte. This enabled the targeted synthesis of its high-conductivity, metastable α -phase. Together, these studies establish a robust design principle for the accelerated discovery and controlled synthesis of advanced materials.

Venue: Auditorium, 1F, NanoGREEN/WPI-MANA Bldg.,
Namiki-site

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