The 92nd GREEN Seminar

Computational materials discovery in the age of AI and robotics

Chair: Dr. Marcela Calpa (GREEN)

Dr. Wenhao Sun

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In the modern age of data science, there is more catalogued and query-able data than ever before. Here I will discuss how we can leverage high-throughput materials data from computational, experimental, and literature sources to accelerate the discovery of new functional materials. First, I will present a large stability map of the ternary metal nitrides, constructed using a suite of high-throughput computational materials discovery and informatics methods. Guided by our map, we experimentally realized a new class of ternary nitride semiconductors with tunable optoelectronic properties, expanding the palette of nitride semiconductors beyond Al/Ga/In-Nitrides. To more effectively design synthesis routes to computationally-predicted materials, we next demonstrate how Natural Language Processing algorithms can extract materials synthesis recipes from the scientific literature. By analyzing trends and anomalies in these published synthesis recipes, we hypothesized new design principles for highly-reactive precursors to complex multicomponent oxides. Using a robotic inorganic materials synthesis laboratory, we show that our predicted precursors substantially outperform traditional precursors. Robotic laboratories offer an exciting new platform for data-driven experimental synthesis science, from which we can develop new fundamental insights to guide both human and robotic chemists.

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

Date: Friday, July 7th, 2023

Time: 14:00-15:00

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