Materials Science and Engineering Department

Winter Seminar Series

Guiding Materials Discovery Using Reaction Informatics

Prof. Alex Norquist
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Haverford College

February 7, 2024
11AM-12PM | Hill Seminar Room (LeBow 240)

Inorganic–organic hybrid materials have been studied for decades, and hydrothermal and solvothermal syntheses have produced thousands of new materials that collectively contain nearly all the metals in the periodic table. The development of new compounds relies primarily on exploratory syntheses because their formation is not fully understood. Simulation- and data-driven approaches provide an alternative to experimental trial-and-error. In this work, an alternative approach that uses machine-learning algorithms trained on reaction data to predict reaction outcomes for the crystallization of both metal oxides and metal halides is demonstrated. Physicochemical property descriptions were generated using cheminformatics techniques, and the resulting data were used to train a machine-learning model to predict reaction outcomes such as crystallite size and structure class. Effects associated with common biases in syntheses were explored in the context of both traditional and high throughput experimentation routes.

Alex Norquist, Professor of Chemistry at Haverford College, earned his BS at Gustavus Adolphus College. His graduate work at Northwestern University, in the lab of Ken Poeppelmeier, was focused on the discovery of noncentrosymmetric metal oxide fluorides. He was a post doc in Dermot O'Hare's lab at the University of Oxford, studying reaction dynamics of hydrothermal syntheses using in situ energy dispersive X-ray diffraction techniques. He has been in the chemistry department at Haverford College since 2003, during which time his research has been largely focused on materials discovery in a wide range of organic-inorganic hybrid materials. More recent work involves the use of both machine learning approaches and high throughput experimental routes.

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