NSF NANOSCALE SCIENCE AND ENGINEERING GRANTEES CONFERENCE:
NANO AND AI CONVERGENCE
DECEMBER 9-10, 2024

"Guiding materials discovery using reaction informatics"

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Bio: Alex Norquist is a Professor in the Department of Chemistry at Haverford College. He received his BS from Gustavus Adolphus College and PhD from Northwestern University, followed by a postdoc in the Inorganic Chemistry Laboratory at Oxford University. He began his academic career at Haverford College in 2003. His research interests are focused on the synthesis of new solid state materials with desirable physical properties. Specific emphasis is placed on the intersection of exploratory syntheses and machine learning in materials discovery. Additional interests involve exploiting synergies between machine learning and automated robotic platforms. Dr. Norquist has received numerous awards, including being named a Henry Dreyfus Teacher Scholar. Dr. Norquist has authored not-quite 100 peer reviewed publications, and served two terms as an elected Councilor in the Council on Undergraduate Research.

Abstract: 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.