DEPARTMENT OF PHYSICS AND ASTRONOMY

CONDENSED MATTER SEMINAR

Friday, December 1, 2017

3:30 PM, Room 203 Physics

Refreshments 3:00 PM Room 242 Physics

Professor Alex Norquist

Haverford College

Materials Discovery Using Machine Learning

Inorganic–organic hybrid materials such as organically templated metal oxides, metal–organic frameworks (MOFs) and organohalide perovskites 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 (promoted by efforts such as the Materials Genome Initiative) 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 templated vanadium selenites is demonstrated. Archived 'dark' reactions, both failed and successful attempts at hydrothermal syntheses, were used to create a database. Physicochemical property descriptions to the raw notebook information using cheminformatics techniques, and the resulting data were used to train a machine-learning model to predict reaction 'success.' When carrying out hydrothermal synthesis experiments using previously untested, commercially available organic building blocks, the machine-learning model outperformed traditional human strategies, and successfully predicted conditions for new organically templated inorganic product formation with a success rate of 89 per cent. Inverting the machine-learning model reveals new hypotheses regarding the conditions for successful product formation.