Joint Materials & Inorganic Seminar

Professor Jakoah Brgoch

University of Houston
Department of Chemistry

"Machine learning-directed search for sustainable ultraincompressible, high hardness materials"

High hardness materials are widely employed in the automotive, aerospace, oil and gas, and manufacturing industries for drilling, cutting, and grinding among other uses. In our pursuit of new materials with exceptional mechanical properties needed for these applications, we have developed a machine-learning model to predict the elastic constants of inorganic materials, which acts as a proxy for hardness. Screening 118,287 compounds compiled in inorganic crystal structure databases using a support vector machine regression analysis, we identified two compounds of interest, a ternary rhenium tungsten carbide and a quaternary molybdenum tungsten borocarbide. These materials are predicted to have an optimum bulk and shear modulus indicating potential high hardness. Both compounds were synthesized using arc melting and characterized using X-ray diffraction and electron microscopy. Subsequent high-pressure diamond anvil cell measurements confirm the accuracy of the machine learning predicted bulk modulus, while Vickers microindentation measurements reveal have a hardness exceeding of 40 GPa at low loads, approaching the superhard regime. Despite the promising mechanical response, the transition metals employed are extremely expensive and scarce starting material hindering their potential for large-scale application. Therefore, our research has also developed a process for using high-information density plots to target new earth-abundant mechanical materials. This method is ideal to quantitatively balance mechanical response with sustainability ensuring only viable compositions are pursued for future development.

Host: Prof. Danny Fredrickson

Thursday
May 2, 2019

12:15 p.m.
1315 Chemistry

Coffee & cookies
at 12 p.m.

DEPARTMENT OF
Chemistry
UNIVERSITY OF WISCONSIN–MADISON