



Hosted by Darren Johnson
& Chris Hendon

Dept. of Chemistry and Biochemistry

Organic/Inorganic Seminar Series

Jakoah Brgoch

University of Houston

Friday, October 19, 2018

2:30–3:30 pm, 331 KLA

Coffee reception @ 2:00 pm, 377 KLA

***Machine learning directed search for sustainable
ultrahard, high hardness materials***

Abstract: 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've 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.

BIO: Prof. Brgoch completed his bachelors and masters in Chemistry from Illinois State U. followed by his Ph.D. from Iowa State U. under the supervision of Gordon Miller. Following postdoctoral research at the U. of California, Santa Barbara in the Materials Research Lab, Jakoah joined the Department of Chemistry at the Univ. of Houston. Jakoah is now leading a multidisciplinary research group with research topics ranging from the development of persistent luminescent materials for bio-imaging to understanding the mechanical response in superhard materials all through a combination of materials synthesis, characterization, first-principles computation, and machine learning.