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# TcSUH Bi-Weekly Seminar

## Machine learning directed search for sustainable ultraincompressible, high hardness materials



### Prof. Jakoah Brgoch

Department of Chemistry; TcSUH PI

**Thursday, October 10<sup>th</sup>, 2019**

Room 102, Houston Science Center

12:00 p.m. – 1:00 p.m.

**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 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.

**BIO:** Prof. Jakoah Brgoch completed his bachelors and masters in Chemistry from Illinois State University followed by his Ph.D. from Iowa State University under the supervision of Gordon Miller. Following postdoctoral research at the University of California, Santa Barbara in the Materials Research Laboratory, Jakoah joined the Department of Chemistry at the University 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.

**RSVP** by Wednesday at noon to [bdherndo@central.uh.edu](mailto:bdherndo@central.uh.edu) for Vietnamese sandwiches.

*Persons with disabilities who require special accommodations to attend this lecture should call (713) 743-8213.*

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