10th TcSUH STUDENT/POSTDOC SEMINAR

Friday, March 7, 2022 - 5:00 pm, HSC 102

RSVP: Food and soft drinks will be served!!

Retaining Superconducting Phases Through Low-Temperature Pressure Quenching

Trevor Bontke

TcSUH and Department of Physics

Abstract: Superconductors are most well-known for allowing electrons to move with zero resistance. These materials have a wide range of applications including magnetic resonance imaging (MRI), lossless energy transmission, maglev trains, quantum computing, and energy storage. One of the main challenges to the widespread implementation of superconducting technologies is the required cryogenic cooling as it is a phenomenon observed below a critical temperature (T_c), typically at temperatures well below -200° C (73 K). Recently, a new class of superconductor called superhydrides was discovered. These materials exhibit superconductivity at room temperature under pressures roughly 2/3 that of the Earth's core (~260 GPa). Such high pressures are impractical for commercial use of room-temperature superconductivity (RTS). For this reason, we developed a technique to apply and then remove the applied pressure to ambient (~1 atm) at cryogenic temperatures. This pressure-quenching technique succeeded in retaining T_cs higher than those observed at ambient pressure in the materials Bi and also FeSe and $Cu_xFe_{1-x}Se$. In the case of $Cu_xFe_{1-x}Se$, we were able to induce and retain superconductivity despite being non-superconducting at ambient pressure. Furthermore, the retained superconducting phase of CuxFe1-xSe exhibited perfect stability for at least a week when kept in the cryogen liquid nitrogen. This work gives some hope that other materials, such as the superhydrides, may be able to remain a RTS after undergoing pressure treatment.

Bio: Mr. Trevor Bontke is currently a Ph.D. candidate in Dr. Paul Chu's group in the Department of Physics and Texas Center for Superconductivity at the University of Houston.

Finding Superhard Materials through Machine Learning

Ziyan Zhang

TcSUH and Department of Chemistry

Abstract: Finding new superhard materials with a Vickers hardness (HV) greater than 40 GPa has traditionally been guided by empirical design rules derived from classically known materials like diamond, c-BN, and more recently ReB_2. A material's Vickers hardness varies with the load applied to the indenter tip, referred to as the indentation size effect. In every measurement, the hardness decreases asymptotically as the load increases, and the origin and the mechanism of the indentation size effect are not well understood. As a result, even if a method can predict a material's hardness at a single load, it is not likely to capture the load-dependent response. This remains a significant barrier in superhard materials design. To address this challenge, we constructed a supervised machine learning model capable of directly predicting load-dependent hardness based only on chemical composition. Ensemble learning algorithms, including Gradient Boosting (GB) and XGBoost (XGB) trees, are employed to maximize the sparse hardness data collected from the literature. The predictive power of our model was first validated using eight unmeasured metal disilicides. Additionally, several classic high hardness materials were also predicted, and these results showed a remarkable reproduction of the Vickers hardness at various loads. The trained model was then used to screen ~66,000 known compounds in Pearson's Crystal Data (PCD) set and combined with our recently developed machine-learning phase diagram tool to identify more than ten previously unreported high hardness compounds. Moreover, we extend the capability of machine learning towards unsupervised learning methods that can be applied on unlabled crystal structure data. We created a novel framework for superhard materials design using artificial neural networks (ANN), more specifically the autoencoder architecture that encodes and reconstructs crystal-chemical representations. Establishing the origin of reconstruction loss will help us design novel materials with exceptional mechanical properties. Both supervised and unsupervised discovery method are poised to modernize the search for new superhard materials benefiting from the efficient, scalable, and transferable nature of machine learning.

Bio: Ms. Ziyan Zhang is currently a Ph.D. candidate in Dr. Jakoah Brgoch's group in the Department of Chemistry and Texas Center for Superconductivity at the University of Houston.

RSVP: BY 4:00 p.m. on THURSDAY, MARCH 3, to tcsuhstudents@uh.edu

Persons with disabilities who require accommodations to attend this seminar should call 713-743-8213.