Materials Discovery through Machine Learning: Experimental Validation and Interpretable Models

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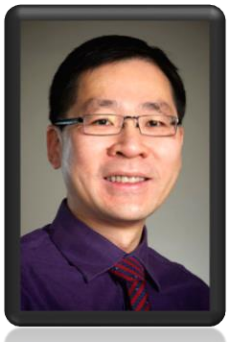

Chemistry Colloquium on *Materials Discovery Through ML*

3:15 p.m.
Friday
Aug 26 in 126 Schrenk

Please contact Dr. Amitava Choudhury at choudhurya@mst.edu for more information

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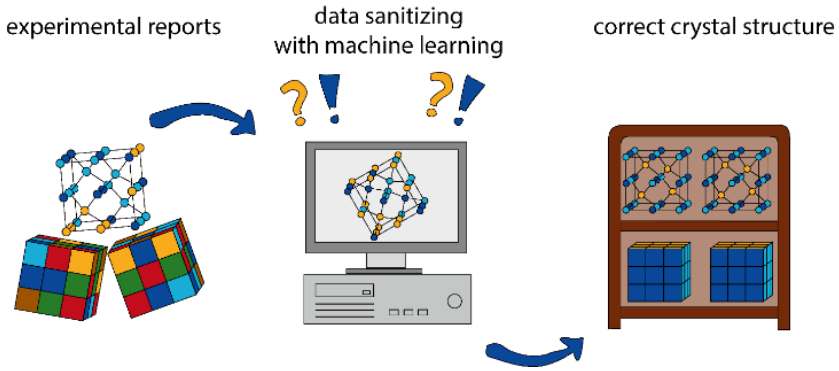
Abstract: Machine learning algorithms have been applied successfully in many areas of materials chemistry. An ongoing challenge is to make accurate predictions of the crystal structures of inorganic solids, their site preferences, and their physical properties. We have previously developed machine learning models to predict structures within the large family of intermetallic compounds known as Heusler compounds (used as thermoelectric materials, ferromagnets, magnetocaloric materials, and catalysts), followed by experimental validation. Nevertheless, skeptics rightfully criticize many of these models as being too "black box," with little chemical insight and explainability. We demonstrate our efforts to generate more interpretable machine learning models, using the structures of binary rare-earth intermetallics *RX* as an example, to illustrate that it is possible to gain insight and practical guidance to prepare new materials.



About the speaker: Dr. Arthur Mar received a Ph.D. from Northwestern University in 1992 under the supervision of James A. Ibers. He worked as an NSERC Postdoctoral Fellow in the laboratory of Yves Piffard and Jean Rouxel at the Institut des Matériaux de Nantes in 1993–1994. He is currently a full Professor in the Department of Chemistry at the University of Alberta. He is a leading expert in inorganic solid state chemistry, with significant contributions in synthesis (intermetallics, Zintl phases, pnictides, chalcogenides), characterization (X-ray diffraction, XPS, physical properties), and applications (magnetic, thermoelectric, superconducting, optical materials). In recent years, he has been at the forefront of applying machine-learning approaches to materials discovery. He has published >230 articles and given >120 invited presentations. He has served on the editorial boards of *Chemistry of Materials*, *Journal of Solid State Chemistry*, and *Acta Crystallographica*. He has received the Faculty of Science Research Award and many teaching awards at the University of Alberta. He is vice-chair (2022) and chair-elect (2024) for the Gordon Research Conference in Solid State Chemistry.