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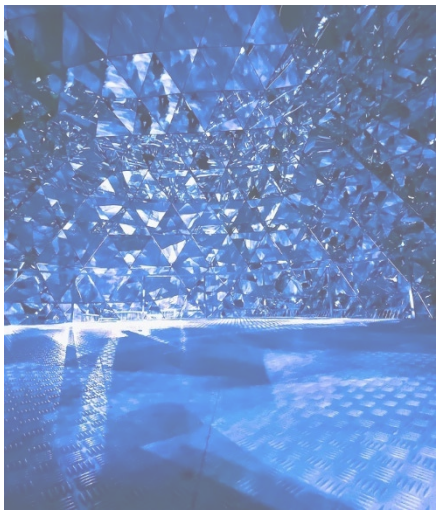
Data-driven materials design in the quantum regime

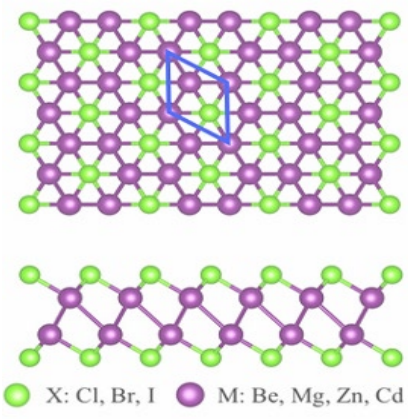
Professor Qimin Yan, Temple University

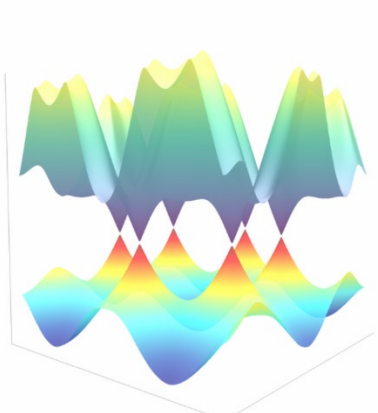


Tuesday, March 29, 2022
3:00 to 4:00 p.m.

Zoom meeting link:
https://northeastern.zoom.us/j/93346146592

Materials design in the quantum regime calls for the integration of multi-tier materials information that goes beyond atomic structures since quantum behavior is often controlled by local symmetries and bonding environment. I will discuss how machine learning and data-driven approaches can be combined with physical principles to accelerate the discovery and design of solid-state quantum materials. Motivated by Pauling's rules, I will show that local bonding environments (motifs) can be incorporated in a graph-based machine-learning architecture to make reliable property predictions for quantum materials including complex metal oxides. The proposed atom-motif dual network model demonstrates the feasibility of incorporating beyond-atom materials information in a graph network framework and achieves a state-of-the-art performance for predicting electronic properties. I will discuss how data-driven materials science can be combined with symmetry-based physical principles to guide the search for exotic topological phases and quantum defects in two-dimensional materials and their heterojunctions for quantum information processing, quantum sensing and other applications.





Dr. Qimin Yan is an Assistant Professor of Physics at Temple University. He received his Ph.D. in from University of California, Santa Barbara in 2012. From 2013 to 2016, he was a postdoctoral researcher at Lawrence Berkeley National Lab and University of California, Berkeley. In 2016, he joined the Department of Physics at Temple University as an Assistant Professor. His current research interests include machine learning and data-driven discovery of solid-state quantum materials, quantum defects for quantum sensing, computing and information technologies, and functional semiconductors for energy conversion. He received the DOE Early Career Award in 2019 and the NSF CAREER Award in 2022.