Ferroic Materials: Designed and Probed using Electrons

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Abstract: Advances in supercomputing capabilities and electronic structure calculations based on density-functional theory (DFT) now make it possible to design materials with new properties starting from the atomic scale, and guide their experimental synthesis and characterization. Concurrent advances in scanning transmission electron microscopy (STEM) enable imaging and spectroscopy of materials with unprecedent spatial and energy resolution. Naturally then, the combination of theory and microscopy provides an unparalleled probe to unravel the atomic-scale structure-property correlations in complex materials with defects and disorder. In this presentation, I will discuss my group's efforts to develop new ferroic materials with defects and disorder for energy and optical applications. Examples will include the discovery of chalcogenide perovskites with colossal optical anisotropy [1,2], unraveling the origin of ferroelectricity in nanoscale hafnia [3]; and the realization of a relatively understudied class of multiferroic that combines ferroelectricity and chirality [4].

Bio: Rohan Mishra is an Associate Professor of Mechanical Engineering & Materials Science, and Physics (by courtesy) at Washington University in St. Louis. He is also an affiliate faculty at the Institute of Materials Science & Engineering at Washington University, where he serves as the Director of Graduate Studies. From 2012-2015, he was a postdoctoral researcher in the Scanning Transmission Electron Microscopy group at Oak Ridge National Laboratory with a joint-affiliation from the Department of Physics at Vanderbilt University. He has a Bachelor in Technology in Metallurgical and Materials Engineering from National Institute of Technology Karnataka in India (2008) and a PhD in Materials Science and Engineering from The Ohio State University (2012). He leads the Materials Modeling and Microscopy group (mcube.wustl.edu) that works on establishing quantitative structure-property correlations in materials using a synergistic combination of electronic structure theory and electron microscopy. Their end goal is the rational design of materials with properties tailored for various energy applications. Mishra has coauthored over 100 journal articles. He received the NSF CAREER award in 2022.

References:

[1] B. Zhao *et al.*, Advanced Materials **36**, e2311559 (2024).
[2] H. Mei *et al.*, Advanced Materials **35**, e2303588 (2023).
[3] X. Li *et al.*, 2024), p. arXiv:2408.01830.
[4] G. Ren *et al.*, Advanced Functional Materials (2024).