Database-Driven Discovery of New Ferroics using First-Principles Methods

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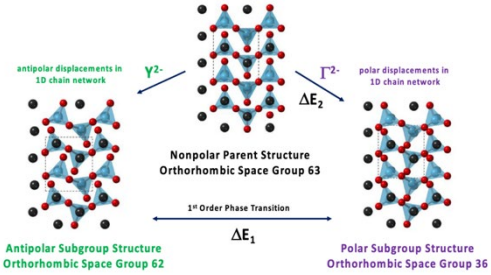
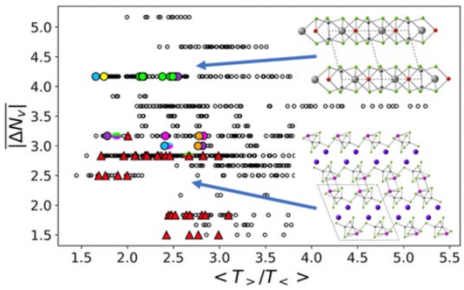
The design and discovery of new materials to be used as platforms for ferroic properties can be expedited by investigating already synthesized and characterized compounds whose merits may have been previously overlooked. Here we use a database-driven methods that combine searchable databases, applied crystallography, group theory, and first-principles density functional theory calculations to create new materials to function over a wide range of chemical environments. First, we investigate a family of known A_2BX_3 compounds as solid state materials for solar harvesting and energy storage, and then use inorganic chemistry and group theory to explain how distortions in the 1D chains present in the structure types can lead to the microscopic mechanisms of ferroelectricity and antiferroelectricity that we predict. Second, we create crystallographic maps of 2D van der Waals layered materials and elucidate which phase spaces could hold promising candidate ferroics. The atomic descriptors presented here can be used to inform neural networks, creating a targeted tool for materials discovery. Taken altogether, these methods lead to new examples of ferroic materials and can be used to guide synthetic routes.





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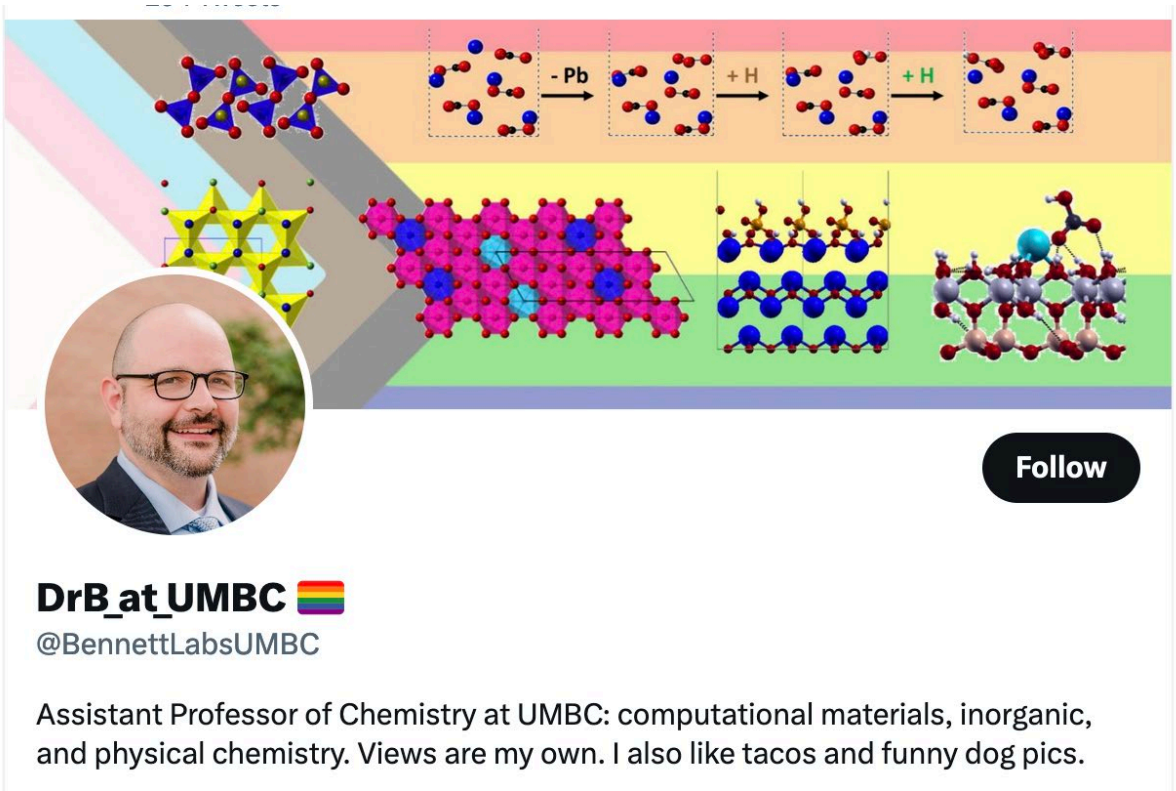

Joe has been at UMBC since 2019, where he spent two years as a pre-faculty fellow before being promoted to Assistant Professor in 2021. Joe's interests span computation and synthesis, and he is passionate about workforce development via training student researchers at all levels of experience. His lab designs new ferroic materials and investigates mineral oxide surface transformation thermodynamics. During the summer he trains students interested in art conservation science how to use DFT methods. (short)

He attended Drexel University and obtained a B.S. in chemistry, where his undergraduate student research was in the field of bio-inspired inorganic chemistry and his education outreach was sponsored by the Science in Motion program. In 2003 he began research as a graduate student at the University of Pennsylvania, working under the co-mentorship of Prof. Andrew M Rappe (Chemistry) and Prof. Peter K. Davies (MSE) to uncover how defects and changes in composition could affect perovskite materials. After obtaining his Ph.D. in Chemistry, his postdoctoral work with Prof. Karin M. Rabe of Rutgers Physics and Astronomy was devoted to mapping out underexplored structure types as functional materials, research that he continues to this day. He then spent a decade in industry, as a consultant, and then as a Research Specialist at the University of Iowa, working with Sara E. Mason, now of Brookhaven National Lab. (long)