From Symmetry to Function: Universal Distortion Principles Guiding Perovskite Optoelectronic Design

Mikhail V. Talanov[1], * Ekaterina G. Trotsenko [1], Leon A. Avakyan[2]
[1] Moscow Institute of Physics and Technology, Dolgoprudnyy, Russia
[2] Southern Federal University, Rostov-on-Don, Russia
*email: mvtalanov@gmail.com

Key words: perovskites, group theory, structural distortions, band gap, improper ferroelectricity

Perovskite-structured crystals represent the most abundant and technologically important class of functional materials, exhibiting a wide range of attractive optical, dielectric, ferroelectric, and other physical properties. While effective structural descriptors are essential for accurate structure prediction, rational materials design, and understanding structure-property relationships, their selection remains particularly challenging in systems with many degrees of freedom. Although Landau's order parameter concept in phase transition theory connects all crystal degrees of freedom, its variation is often interpreted merely as a system's response to external stimuli, restricting its broader utility in materials science.

In this work, we introduce a novel approach that bridges symmetry-derived order parameters as structural descriptors with fundamental materials chemistry principles. We demonstrate the universality of composition-driven atomic displacements in distorted *Pnma* perovskites, a family of high technological relevance. Our findings reveal that fundamental symmetry relations, governed by group-theoretical descriptors, depend primarily on distortion magnitude rather than specific chemical composition. This insight enables clear correlations between these descriptors and classical chemical bonding characteristics, such as electronegativity, thereby extending Landau's order parameter framework into chemical space and offering a new paradigm for structure-property analysis.

To validate our approach, we integrate group-theoretical methods with quantum mechanical calculations, highlighting two practical applications: (1) bandgap tuning in halide perovskites and (2) superlattice design in hybrid improper ferroelectrics. Furthermore, our methodology successfully classifies chemically diverse systems (oxides, fluorides, halides, and chalcogenides) by linking structural descriptors to bonding behavior. These results underscore the versatility of symmetry-derived descriptors and pave the way for advanced materials discovery not only in perovskites but across broader material families.

The study was supported by the Russian Science Foundation grant No 22-72-10022 (group theory, DFT calculations) and the Ministry of Science and Higher Education of the Russian Federation grant No 075-15-2025-010 (structure-property relations).