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Shedding Light on the Structure-Property Relationship through Representation Analysis

The research objective of this project is to develop group-theoretical tools that will make use of the existing tabulation of the irreducible representations of the 230 space-groups, in order to study phase transitions in functional materials.

Background: Most matter is crystalline and its structure can be described by one of the 230 space groups. In addition to being an invaluable tool for describing the structure of matter, classifying structure in terms of symmetry has allowed physicists and chemists to rationalise the physical properties of many functional materials. As every physical property can be described by a tensor, which itself transforms under a specific set of symmetry operators related to those of the structural space group symmetry, this allows for a certain level of abstraction when trying to design new materials exhibiting certain desired properties. However, many physical properties arise due to solid state to solid state phase transitions, in which a structure described at higher temperatures by a particular "parent" space group undergoes a transition to another structure, which can now only be described by a "child" space group which is a subgroup of the parent. The "order parameter" for the phase transition, the set of continuous atomic or electronic displacements driving this lowering of symmetry, is restricted to transforming as an irreducible representation of the parent space group (harmonic approximation). Classifying order parameters in terms of irreducible representations of the parent symmetry is hence an important step to understanding the structure-property relationship, and has been used to great effect to understand magnetic, ferroelectric and multiferroic properties. These properties can all be understood in terms of arrangements of electric (polar vectors) and magnetic (axial vector) dipoles that transform according to particular irreducible representations of the possible parent space group. However, some physical properties such as superconductivity are related to electronic densities and wave functions that do not transform simply as dipoles, but instead as higher order multipoles. Here, currently no tools exist to ascertain which irreducible representation (of the space group) these higher order multipoles transform as – and hence the order parameters for these phase transitions are not easily formally classified.

Prospective Deliverables: By the end of the project it is hoped that the candidate will develop an algorithm for classifying which pre-tabulated irreducible representation of a given parent space group describe the symmetry breaking associated with multipolar order of an arbitrary order.

Real World application: This project will deliver research tools for the large number of scientists involved in studying phase transition in the solid state, that are relevant to understanding technologically important properties such as magnetism, superconductivity and the thermoelectric effect.

Extension to PhD: The project will be extended to form a full PhD as follows. The tools developed for studying multipolar order will be used to analyse the large structural databases that exist for known organic and inorganic compounds, shedding light onto what extent many of these phase transitions (and hence resulting physical properties) can be described by multipolar order. In tandem, the tool will be used in a predictive manner, exploring how different kinds of multipolar order can be coupled together to control specific physical properties. The student will gain an understanding of invariants analysis and Landau-Ginzburg theory, and will ultimately apply this knowledge to studying phase transitions related to high temperature superconductivity in the layered cuprates.

Further Reading:

Senn, M.S. (2017). *Acta Cryst.* **A73**, 1–3.
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Howard, C. J. & Stokes, H. T. (1998). *Acta Crystallogr. Sect. B Struct. Sci.* **54**, 782–789.