# Reports on MERIT internship

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## Period of acceptance

2021/08/16~2022/02/10

## Place (Supervisor)

National Institute of Material Science (Dr. Terumasa Tadano)

## Research topic

Development and application of structural optimization at finite temperatures based on the self-consistent phonon theory.

## Background

In recent years, first-principles electronic structure calculations, such as DFT (density functional theory), plays an important role in computational material science. These electronic structural calculations require the crystal structure as an input, and it is important to predict the crystal structure non-empirically. In crystal structure calculations, DFT-based crystal structure optimization is often used, but it has the disadvantage that it cannot incorporate finite temperature effects. In addition, the current methods that can incorporate finite temperature effects are computationally heavy and cannot be applied to complex materials. Therefore, there is a need to develop a computational method that can efficiently obtain the crystal structure at finite temperature for a wide range of materials.

## Research

In this study, we extend the self-consistent phonon (SCP) theory, which is an anharmonic phonon theory, to formulate and develop a calculation method for crystal structure optimization at finite temperatures. We implemented the obtained theory in ALAMODE, a package for anharmonic phonon calculations, which was developed by Dr. Tadano, who gave me advices on various aspects of the formulation and implementation.
Using the implemented program, we calculated the most representative ferroelectric material, $BaTiO_3$, and succeeded in reproducing the three-step sequential phase transition from cubic to tetragonal to orthorhombic to rhombohedral. The temperature dependence of the lattice parameter and polarization was also reproduced with high accuracy.

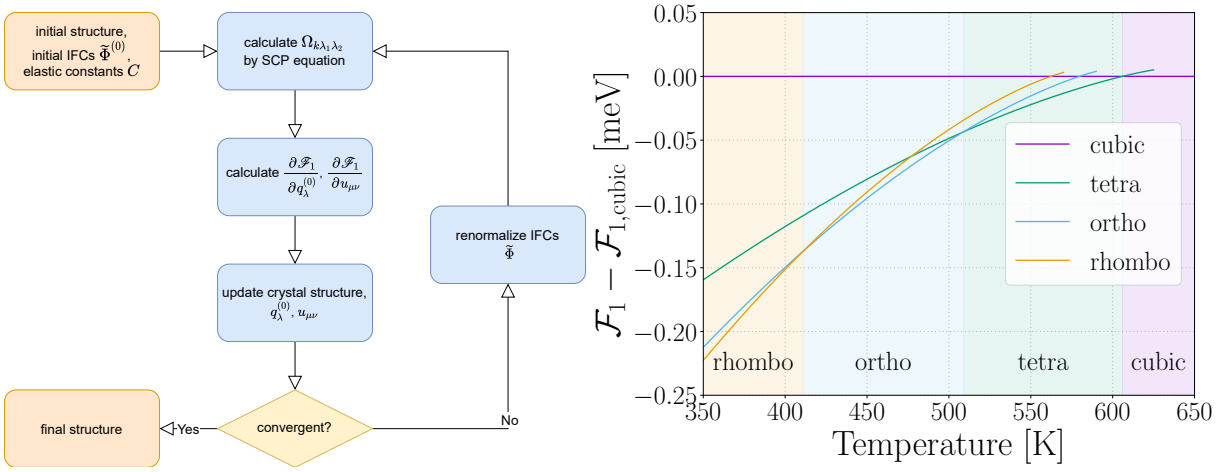


Fig.1 (left) The calculation scheme of structural optimization at finite temperature. F is the SCP free energy. $\Omega$ is the SCP frequency, u and q are strain and atomic shift. (right) The temperature dependence of SCP free energy of the four phases of $BaTiO_3$.

## Acknowledgment

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