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Science Research Bldg. 1, 4th floor.
Ehime Univ.

Keywords:
1. High pressure
2. Fluoroperovskites
3. Crystal-structure prediction

High-Pressure Pathways in Na-Based Fluoroperovskites: From Perovskite to Post-Perovskite and Beyond

Sodium fluoroperovskites $NaMF_3$ provide model systems for investigating pressure-induced structural transformations at experimentally accessible conditions. In these compounds, compression can drive the reconstructive transformation from the three-dimensional corner-sharing perovskite framework to the layered post-perovskite structure, offering a useful analogue to transitions occurring in mantle silicates.

In this seminar, I will present our recent experimental and computational work on several Na-based fluorides. $NaFeF_3$ provides a benchmark system in which the post-perovskite phase can be recovered after high-pressure/high-temperature treatment. This structural rearrangement strongly modifies the connectivity of the FeF_6 octahedra and also affects the calculated Na^+ migration pathways. $NaNiF_3$ highlights the role of microstructure: samples with identical composition but different particle size and morphology exhibit distinct compressional behaviour and transformation kinetics, showing that pressure and temperature alone are not sufficient to describe the Pv-pPv transition.

These experimental studies are complemented by crystal-structure prediction for $NaMnF_3$ and $NaGeF_3$. The calculations reveal competing structural pathways and, in some cases, phases departing from the conventional perovskite/post-perovskite sequence. $NaGeF_3$ is particularly striking, with independent searches predicting layered low-energy structures at both 0 and 15 GPa. Together, these results illustrate how high-pressure experiments and structure prediction can be combined to explore and stabilize new fluoride phases.

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