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Understandng of phonon anharmonicity in thermoelectric clathrates KATSUMI TANIGAKI, JIAZHEN WU, HIDEKAZU SHIMOTANI, KHUONG HUYNH, KAZUTO AKAGI, Tohoku University, AIMR COLLABORATION, DEPARTMENT OF PHYSICS, GRADUATE SCHOOL OF SCIENCE COLLABORATION — Anharmonicity in phonons, apart from the conventional Einstein- or Debye- mode harmonic phonons, is frequently observed for amorphous or glass-like materials. A frontier topic relating to anharmonic phonons revolves around the fact that they are also observed in a single crystal with a void of cage structure. Although the origin of the phonon anharmonicity has been the center of scientific debate for many years, a clear understanding has not yet been achieved. In the present study, we show that the anharmonic oscillations in thermoelectric clathrates can successfully be rationalized in terms of a single unified exponential line for a variety of clathrates by employing a new parameter associated with the freedom of space. The intrinsic nature of phonon anharmonicity is described based on the unified picture with a help of first principles calculations. Although the origin of the anharmonicity appearing in disordered materials is complex to understand due to the missing information on the real structure, the present unified picture gives important information applicable to other systems.

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