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Author

Nakayama T.　　Kaneshita E.

Tittle

Significance of Off-Center Rattling for Emerging Low-Lying THz Modes in Type-I Clathrates

Source

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN vol. 80 no.10 104604 DOI: 10.1143/JPSJ.80.104604 OCT 2011

Abstract

We show that the distinct differences of low-lying THz-frequency dynamics between type-I clathrates with on-center and off-center guest ions naturally follow from a theoretical model taking into account essential features of the dynamics of rattling guest ions. Our model analysis demonstrates the drastic change from the conventional dynamics shown by on-center systems to the peculiar dynamics of off-center systems in a unified manner. We claim that glasslike plateau thermal conductivities observed for off-center systems stem from the flattening of acoustic phonon dispersion in the regime vertical bar k vertical bar < vertical bar G vertical bar/4. The mechanism is applicable to other systems such as glasses or relaxers.