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摘要: A theory is given of a role of rattling guest ions to the emergence of THz frequency libration modes in type-I clathrates involving off-centered guest ions. We clarify the physical origin of distinct differences on THz frequency dynamics between on-center and off-center systems. It is demonstrated that the spontaneous symmetry breaking of rattling off-centered guest ions is a key for the emergence of low-lying band-modes hybridized with acoustic modes in the THz-frequency range. 
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