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Theory of Thermal Conductivity of Thermoelectric Clathrates above the Plateau QING XI, JUN ZHOU, Center for Phononics and Thermal Energy Science,School of Physics Science and Engineering, Tongji University, 200092,Shanghai, China, TSUNEYOSHI NAKAYAMA, Hokkaido University, Sapporo 060-0826, Japan, BAOWEN LI, Department of Mechanical Engineering, University of Colorado, Boulder, Colorado 80309, USA — Phonon heat transport in structural glasses is one of unsolved problems remained in condensed matter physics. Observed heat transports exhibit universal characteristics, though each glass possesses individual complex microscopic structure. This feature explains the difficulty to identify the microscopic origin. Type-I clathrates with regularly arrayed cage network show identical phonon thermal conductivities to structural glasses, because the guest atoms in cages take disordered configuration. This enables us to identify the structural origin of glasslike thermal properties in type-I clathrates. We demonstrate, by combining with large-scale numerical simulations, that there are three kinds of modes relevant to the emergence of glasslike thermal conductivities. These are extended, weakly and strongly localized vibrational modes. Our formula based on extended-mode-assisted hopping of strongly localized modes satisfactorily explains the magnitude and the temperature dependence of observed thermal conductivities above the plateau.

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