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Exact Thermal Transport Properties of Gray-Arsenic using Electon-Phonon Coupling SEOUNG-HUN KANG, Korea Inst for Advanced Study, YOUNG-KYUN KWON, Kyung Hee University — Using various theoretical methods, we investigate the thermoelectric property of gray arsenic. Thermoelectric devices that utilize the Seebeck effect convert heat flow into electrical energy. The conversion efficiency of such a device is determined by its figure of merit or ZT value, which is related to various transport coefficients, such as Seebeck coefficient and the ratio of its electrical conductivity to its thermal counterpart for given temperature. To calculate various transport coefficients and thus the ZT values of gray arsenic, we apply the Boltzmann transport theory to its electronic and phononic structures obtained by density functional theory and density functional perturbation theory together with maximally locallized Wannier functions. During this procedure, we evaluate its relaxation time accurately by explicitly considering electron-phonon coupling. Our result reveals that gray arsenic may be used for a good p-type thermoelectric devices.

Seoung-Hun Kang
Korea Inst for Advanced Study

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