

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Thermoelectric property of a new silicon crystal KISUNG CHAE, SEON-MYEONG CHOI, Korea Inst for Advanced Study, DUCK YOUNG KIM, Carnegie Institute of Washington, YOUNG-WOO SON, Korea Inst for Advanced Study — We present ab initio calculations on thermoelectric properties of a recently synthesised allotrope of silicon crystal [1]. A new silicon crystal with 24 Si atoms per unit cell has open channels along the specific crystallographic direction and shows a quasidirect energy gap of 1.3 eV. Using various first-principles calculation techniques for electrical and thermal conductivity as well as Seebeck coefficient, we find large suppression of thermal conductivity and relatively large Seebeck coefficient in the new silicon crystal, thus demonstrating a competitive thermoelectric figure of merit. [1] D. Y. Kim et al, Nat. Mat. 14, 169 (2015).

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Date submitted: 05 Nov 2015

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