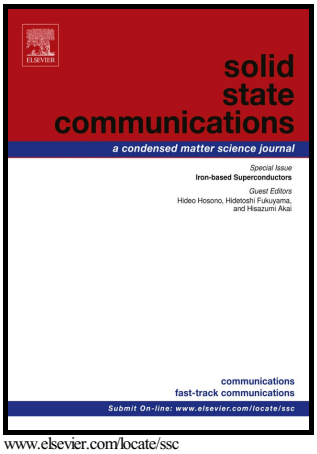

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Lattice dynamics and thermal conductivity of cesium chloride via first-principles investigation

Cui He [1], Cui-E Hu [2], Tian Zhang [1], Yuan-Yuan Qi [3], Xiang-Rong Chen [1*]

[1] Institute of Atomic and Molecular Physics, College of Physical Science and Technology, Sichuan University, Chengdu 610065, China

[2] College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047, China

[3] College of Science, Henan University of Technology, Zhengzhou 450001, China

[*]Corresponding author. xrchen@scu.edu.cn

Abstract

The lattice thermal conductivity of CsCl crystal is theoretically investigated from a first-principles theoretical approach based on an iterative solution of the Boltzmann transport equation. Real-space finite-difference supercell approach is employed to generate the harmonic and anharmonic interatomic force constants. Phonon frequencies, velocities, and specific heat capacity as well as anharmonic properties are then obtained and applied to calculate the bulk thermal conductivity of CsCl crystal at the temperatures ranging from 20 K to 700 K. The calculated lattice thermal conductivity 1.14 W/mK of CsCl at room temperature agrees well with the experimental value, demonstrating that this parameter-free approach can provide a good description for the thermal transport of this material. The RTA and iterative solution of BTE are both presented. Our results show that both methods can obtain the thermal conductivity successfully.

Keywords