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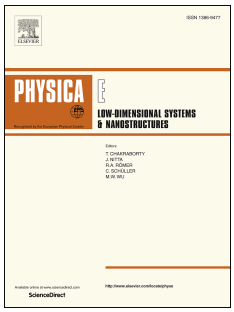

Direction-dependent electronic thermal conductivity and thermopower of single-layer black phosphorus in the presence of bias voltage and dilute charged impurity

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Direction-dependent electronic thermal conductivity and thermopower of single-layer black phosphorus in the presence of bias voltage and dilute charged impurity

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Abstract

By using the Green's function and tight-binding model within the Born approximation, we obtain the electronic thermal conductivity (TC) and Seebeck coefficient [or thermopower (TP)] of monolayer black phosphorus (BP) under charged impurity doping. The results show that the TC and TP of $y-$direction are larger than the $x-$direction in clean BP due to the inherent higher value of the electronic density of states in $y-$direction. Furthermore, the TC linearly decreases with low impurity concentrations in both directions, whereas it decreases and does not change with low impurity scattering potentials in $x-$ and $y-$direction, respectively. On the other hand, TP increases (decreases) with very dilute impurity concentrations and scattering potentials in $x-(y-)$direction. To be a complete work, we also studied these properties in impurity-infected biased BP. We found that the TC of BP in the presence of impurity gradually increases with bias voltage in both directions and TP has a decreasing (increasing) treatment in $x-(y-)$direction. Our findings move the thermoelectric (TE) applications of BP into promising TE materials.

Keywords: Impurity, Green's function, Thermoelectric material, Black phosphorus, Born approximation

1. Introduction

The carbon nanostructures, especially graphene [1, 2], has been significantly studied by a various number of researchers. Developing two-dimensional (2D) materials has enhanced the focus on other nanostructures based on molybdenum, silicon, boron, and phosphorus [3, 4, 5, 6]. Layered transition metal dichalcogenides like MoS_2 represent unique properties that distinguish them from graphene and other 2D structures [7]. Contrary to MoS_2, which has a large direct band gap, graphene is gapless which limits its application in high ON/OFF current ratio [8, 9]. BP, as one of the diverse allotropes of phosphorus, has also attracted great interest due to its inimitable potential in nanoelectronics and optoelectronics. In addition, experiments have reported that BP has a direct gap between 0.35 eV and 2.00 eV [10].

Many research teams recently have synthesized the monolayer BP by utilizing exfoliated bulk BP [11, 12]. BP hybridization is sp^3 formed by a puckered honeycomb lattice structure where each phosphorus atom is covalently bonded to three neighbor atoms. As a new 2D semiconductor, BP displays excellent properties, including high ON/OFF current ratio [13, 14], high carrier mobility [15], mechanical malleability [16], the anisotropic thermal, and electrical conductivity [17], etc. Hence, BP has numerous applications in electronic devices [18, 19] and TE devices [20, 21].

The environmental impact of the global climate change has become increasingly alarming due to the combustion of fossil fuels. Thereby, more than 60% of the produced energy is lost, most in the form of waste heat. One promising approach to increase energy efficiency and thus to reduce greenhouse gas emissions consists in recovering this, otherwise wasted heat using TE materials [22, 23]. Achieving a high efficiency implies increasing TP and electrical conduc-

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