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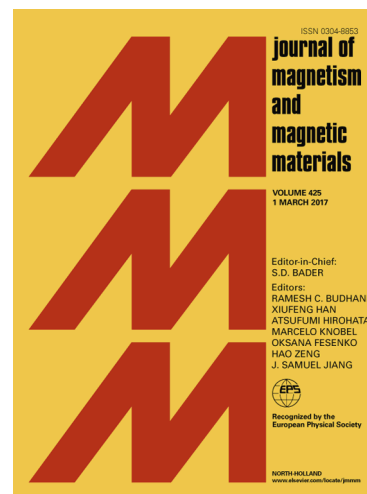
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Direction-dependent electronic phase transition in magnetic field-induced gated phosphorene

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Abstract

A detailed physical meaning of the electronic phase transition in monolayer black phosphorus (BP) has been addressed in the presence of local gate voltage and Zeeman magnetic field. The main features of this transition characterize within the electronic density of states (DOS) in the vicinity of Fermi level. The numerical calculations have been performed within the continuum approximation of tight-binding model and the Green's function method. The anisotropy crystal structure of BP causes different behaviors in each component of DOS. First, we have confirmed the Zeeman effect, i.e. the splitting of Van Hove singularities. Then, our results show that the electronic band gap of phosphorene in the x -direction in the absence of gate voltage decreases with weak magnetic fields and system transits to the semimetallic phase at strong regimes, whereas there is no phase transition in the y -direction. Interestingly, turning on the gate, phase transition independent of the direction does not occur at both weak and strong magnetic fields. Another remarkable point refers to the increase of the band gap with gate voltage at both directions, leading to the semimetallic-semiconductor transition in the x -direction at strong magnetic fields. The controllable band gap with the gate voltage and magnetic field quantities are useful for future applications of BP.

Keywords: Magnetic field, Electronic phase transition, Density of states, Fermi energy, Black phosphorus, Gate voltage

1. Introduction

A reported promising candidate with a direct band gap [1], so-called black phosphorus (BP), is going to be a ON-OFF device instead of gapless graphene. Monolayer BP, a single layer of black phosphorus [2], has been extensively studied recently both theoretically and experimentally [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. Monolayer BP has a band gap of about 1.5-2 eV [1, 13] with large mobility which makes it applicable in real industry. Furthermore, high anisotropy crystal structure of monolayer BP due to the different masses in different directions has attracted great attention of researchers in these years to investigate direction-dependent transport and optical properties of phosphorene.

The perpendicular magnetic field-dependent transport and optical properties of monolayer BP have been reported theoretically in Refs. [14, 15]. Since pristine phosphorene is a nonmagnetic semiconductor, understanding magnetic field effects will provide useful information about electronic and optical properties of this material. In Ref. [14], the different Landau splitting of the conduction and valence bands have been shown due to the anisotropic crystal structure of BP.

In recent years, people controlled the band gap of different shapes of phosphorene by very common ways such as applying electric field [16, 17, 18], doping [19, 20, 21], and hydrogenation [22, 23, 24]. It has been shown that the giant Stark effect occurs depending on the strength and direction of the electric field. Since gate voltage acts like uniform electric field, here, we consider the gate voltage as one of the important factors in gap engineering. Besides this potential, the

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