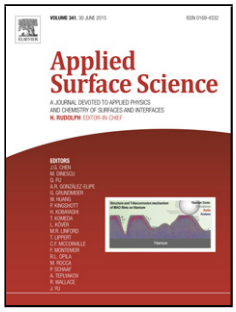

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Tunable Rashba spin splitting in two-dimensional graphene/As-I heterostructures

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Highlights

- Large and tunable Rashba spin splitting can be realized in graphene/As-I van der Waals heterostructures by varying interlayer distance.
- Strong hybridization between C-p_z and As-p_{xy} orbitals.
- Intrinsic built-in electric field in the direction perpendicular to the interface induced by charge redistribution

Abstract

Interlayer distance induced Rashba spin splitting is predicted in graphene and monolayer iodinated arsenene (As-I) van der Waals heterostructures based on first-principle calculations. The equilibrium structure of graphene/As-I exhibits a linear Dirac-like dispersion relation at K point in Brillouin zone. With the change of interlayer distance, large and tunable Rashba spin splitting can be realized from zero to more than 100 meV. Projected band structure analysis is performed, which indicates a strong relation between the extent of band splitting and the hybridization of C and As orbitals near the Fermi level. Meanwhile, charge density difference calculations reveal a pronounce charge transfer between graphene and As-I with varying interlayer distances, leading to the change of built-in electric filed along z direction that modifies the electronic structures significantly. Our work may make a special contribution to the realization and application of spintronic devices based on van der Waals heterostructures.

Keywords: Rashba spin splitting; van der Waals heterostructure; graphene; chemical functionalized arsenene; first-principle calculation

Introduction

Two dimensional (2D) materials with extremely small thicknesses from one to several atomic layers have emerged in different material systems from both elemental substances and compounds since the discovery of grapnene[1, 2]. The unique and superior physicochemical properties of 2D materials are fascinating and have aroused considerable attentions and extensive studies[3, 4, 5]. In recent years, group V elemental monolayers, including black/blue phosphorene6 and arsenene7 are drawing great interest for their promise in practical applications such as field effect transistors8. Pristine arsenene is an indirect band gap semiconductor with a buckled structure, which can be turned into a quasi-palnar layer by different chemical decorations9. Along with the structural transition, significant modification of electronic properties occurred, and chemical functionalized arsenenes are found to be Dirac materials[10, 11] and large band gap quantum spin Hall insulators12. Graphene is known for its K point Dirac cone formed by π bonding of C atoms13. Different from graphene, the Dirac cone in chemical functionalized arsenene is a new σ-type, which is related to the p_{xy} orbitals of As atoms[9]. Thus, it is of great interest to design a heterostructure based on these two nanomaterials and exotic electronic properties can be anticipated.

In 2D condensed matter systems, momentum-dependent splitting of spin bands, Rashba effect, have been demonstrated in semiconductor heterosturctures and surface states of metals[14, 15]. The underlying mechanism of the spin-split electronic states is believed to be the breaking