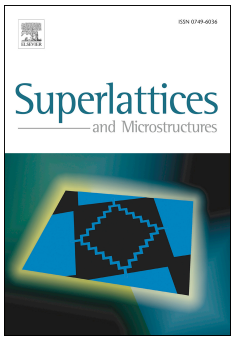
Accepted Manuscript



Effects of interlayer coupling on the electronic structures of antimonene/graphene van der Waals heterostructures

Fang Zhang, Wei Li, Xianqi Dai

PII: S0749-6036(16)30553-5

DOI: 10.1016/j.spmi.2016.10.040

Reference: YSPMI 4585

To appear in: *Superlattices and Microstructures*

Received Date: 25 July 2016

Accepted Date: 17 October 2016

Please cite this article as: F. Zhang, W. Li, X. Dai, Effects of interlayer coupling on the electronic structures of antimonene/graphene van der Waals heterostructures, *Superlattices and Microstructures* (2016), doi: 10.1016/j.spmi.2016.10.040.

Effects of interlayer coupling on the electronic structures of antimonene/graphene van der Waals heterostructures

Fang Zhang [a], Wei Li [b, c,*] and Xianqi Dai [c]

[a] College of Electric and mechanical Engineering, Pingdingshan University, Pingdingshan 467000, China
[b] School of Mathematics & Physics, Henan University of Urban Construction, Pingdingshan 467036, China
[c] College of Physics and Materials Science, Henan Normal University, Xinxiang 453007, China

ABSTRACT

Using density functional theory calculations, we study the electronic structures of antimonene/graphene van der Waals(vdW) heterostructures. It is demonstrated that weak vdW interactions dominate between antimonene and graphene with their intrinsic electronic properties preserved. Furthermore, the n-type Schottky barrier to p-type Schottky barrier transition occurs when the interlayer distance decreases from 5.0 to 3.1Å , which indicates that the Schottky barrier can be tuned effectively by the interlayer distance in the vdW heterostructures. We find that interfacial charge transfer and the Fermi level shift determine the Schottky barrier transition in the antimonene/graphene heterostructure.The present study would open a new avenue for application of ultrathin antimonene/graphene heterostructures in future nano- and optoelectronics.

Keywords: interlayer coupling; Schottky barrier; the electronic structures; antimonene/graphene van der Waals heterostructures

1. Introduction

Two-dimensional (2D) materials, such as graphene, BN, transition metal dichalcogenides (TMDs), and phosphorene, have received considerable attention owing to their excellent mechanical, optical, chemical, electronic and thermal properties which make these materials promising for next-generation nanoelectronic and optoelectronic devices [1-7]. Besides their outstanding properties, they have the potential[1]to lead to drastic reductions in the characteristic lengths of devices [8–10]. Although the most

* Corresponding author.
E-mail address: liwei19801210@126.com (W. Li).