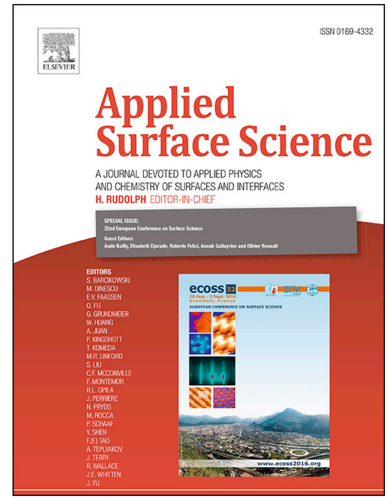
Accepted Manuscript



Full Length Article

Tunable electronic and magnetic properties of antimonene system via Fe doping and defect complex: A first-principles perspective

Shuhua Dai, Wei Zhou, Yanyu Liu, Yi-Lin Lu, Lili Sun, Ping Wu

PII: S0169-4332(18)31095-X
DOI: https://doi.org/10.1016/j.apsusc.2018.04.135
Reference: APSUSC 39134

To appear in: *Applied Surface Science*

Received Date: 26 January 2018
Revised Date: 10 April 2018
Accepted Date: 12 April 2018

Please cite this article as: S. Dai, W. Zhou, Y. Liu, Y-L. Lu, L. Sun, P. Wu, Tunable electronic and magnetic properties of antimonene system via Fe doping and defect complex: A first-principles perspective, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.04.135

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Tunable electronic and magnetic properties of antimonene system via Fe doping and defect complex: A first-principles perspective

Shuhua Dai[a], Wei Zhou[a], Yanyu Liu[a], Yi-Lin Lu[a], Lili Sun[a], Ping Wu[a,*]

Department of Applied Physics, Institute of Advanced Materials Physics, Tianjin Key Laboratory of Low Dimensional Materials Physics and Preparing Technology, Faculty of Science, Tianjin University, Tianjin 300072, People's Republic of China

Abstract

We investigate the electronic and magnetic properties of Fe-doped (Fe_{Sb}) and defect complex (Fe_{Sb} + V_{Sb}) tuned antimonene systems. Our calculations showed that the method of generalized gradient approximation with on-site Coulomb repulsion (GGA+*U*) obtained a larger magnetic moment in the two defect systems than that of generalized gradient approximation (GGA). When the spin-orbit couplings (SOC) effects were turned on, the Fe-doped system transforms from a narrow band-gap semiconductor to a semi-metallic material by the scheme of GGA+*U*. Moreover, the concurrence of strong orbital hybridization (*p*-*d*) and spin-orbit interaction lead to a significant spin splitting around the Fermi level. Especially, stable room temperature ferromagnetism (RTFM) is obtained in Fe-doped systems. However, the system presents anti-ferromagnetism (AFM) order when two intrinsic vacancies (V_{Sb}) are introduced into the Fe-doped systems, which is not conducive to Fe-doped antimonene materials applied in spintronics devices. Comparing with pure antimonene, the relatively flat impurity band indicates lower carrier mobility in Fe_{Sb} + V_{Sb} system. Hence, in Fe-doped antimonene materials, the intrinsic vacancies should

[*] Corresponding author. Tel.: +86-22-27408599
E-mail address: pingwu@tju.edu.cn (P. Wu).

ACCEPTED MANUSCRIPT

Download English Version:

https://daneshyari.com/en/article/7833790

Download Persian Version:

https://daneshyari.com/article/7833790

Daneshyari.com