Pis'ma v ZhETF, vol. 105, iss. 2, pp. 105 – 105 © 2017 January 25

Modulation of band gap by normal strain and an applied electric field in SiC-based heterostructures[1)]

M. Luo[+2)], *Y. E. Xu*[+*], *Y. X. Song*[×]

[+]*Department of Electronic Engineering, Shang Hai Jian Qiao University, 201306 Shanghai, China*

[*]*School of Microelectronic of Fudan University, 200433 Shanghai, China*

[×]*Key Laboratory of Polar Materials and Devices, East China Normal University, 200241 Shanghai, China*

Submitted 24 October 2016
Resubmitted 8 December 2016

DOI: 10.7868/S0370274X17020096

Currently, the van der Waals (vdW) heterostructures comprised of different types of chemically different 2D materials have attracted considerable interest and may have some potential use in future nanoelectronic devices. In order to find its potential applications, we examine the possible modulation of electronic structure of the WS_2/SiC vdW heterostructures (shown in Figs. 1a and b) under the application of normal strain and an external electric field by using first-principles calculations. The first-principles method is based on density functional theory (DFT), which is implemented in the VASP package. Application of the normal strain and the E-field is found to modulate the band gap of the vdW heterostructures. As shown in Fig. 1c, the system has a direct band gap of 1.33 eV at the equilibrium state. The compressive strain has much influence on the band gap of the vdW heterostructures, and the band gap gets an increment to 1.629 eV when the distance is about 2.8 Å. The results of charge density differences and electrostatic potential imply that more electrons are likely to transfer from WS_2 to SiC monolayer. More interesting phenomena are found when an E-field was applied. The band gap first increases and then decreases, which approximatively shows a parabola-like relation with the E-field. As the E-field changes from −0.50 to +0.20 V/Å, on one hand, the band gap reaches a maximum of about 1.90 eV at −0.15 V/Å. On the other hand, the WS_2/SiC bilayer becomes a zero-gap system at −0.50 and +0.20 V/Å, respectively. The band structures and PDOS calculations indicate that different states of W, S, Si, and C atoms contribute to such significant variations of band gap. Remarkably, our results predict that the band gap of the WS_2/SiC vdW heterostructures can be tuned much more effectively by an external electric field. This finding is very important for the potential applications of WS_2/SiC vdW heterostructures in future nanoelectronic devices.

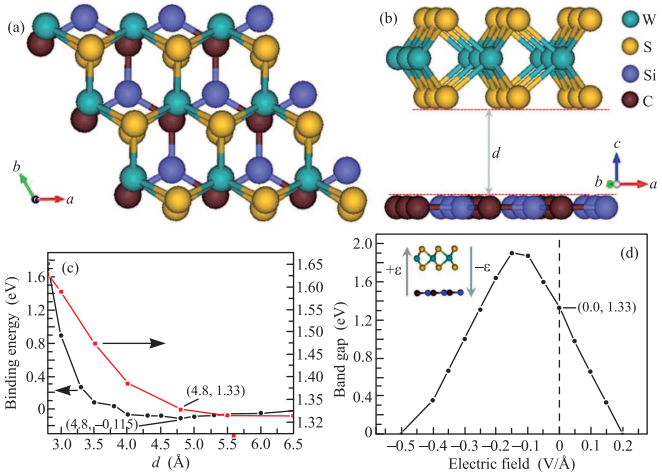

Fig. 1. (Color online) Top (a) and side (b) view of the WS_2/SiC vdW heterostructures, the interlayer distance changes along the c-axis. (c) – Binding energy and energy band gap of the nanocomposite as a function of the interlayer distance. The black circles denote the binding energy and the red squares represent the band gap. (d) – Energy band gap of the nanocomposite as a function of the external electric field

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364017020035

[1)]See Supplemental material for this paper on JETP Letters suit: www.jetpletters.ac.ru.

[2)]e-mail: mluo@gench.edu.cn