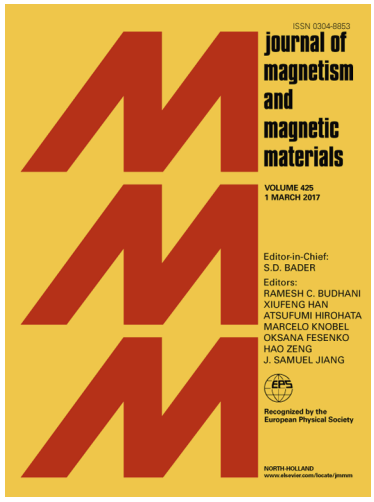

Structural and Electronic Properties of PdS_2 Nanoribbons

Yan Gan, Ruge Quhe, Liyuan Wu, Siyao Hou, Jingyun Bi, Gang Liu, Pengfei Lu

PII: S0304-8853(17)33706-X
DOI: https://doi.org/10.1016/j.jmmm.2018.03.044
Reference: MAGMA 63815

To appear in: *Journal of Magnetism and Magnetic Materials*

Received Date: 28 November 2017
Revised Date: 6 March 2018
Accepted Date: 19 March 2018

Please cite this article as: Y. Gan, R. Quhe, L. Wu, S. Hou, J. Bi, G. Liu, P. Lu, Structural and Electronic Properties of PdS_2 Nanoribbons, *Journal of Magnetism and Magnetic Materials* (2018), doi: https://doi.org/10.1016/j.jmmm.2018.03.044

Structural and Electronic Properties of PdS_2 Nanoribbons

Yan Gan,[1] Ruge Quhe,[2,3*] Liyuan Wu,[2] Siyao Hou,[2] Jingyun Bi,[2] Gang Liu,[1,4*] and Pengfei Lu[2,5*]

[1]*Beijing Key Laboratory of Space-ground Interconnection and Convergence, Beijing University of Posts and Telecommunications, Beijing, 100876, China*
[2]*State Key Laboratory of Information Photonics and Optical Communications, Beijing University of Posts and Telecommunications, Beijing 100876, China*
[3]*School of Science, Beijing University of Posts and Telecommunications, Beijing 100876, China*
[4]*Century College, Beijing University of Posts and Telecommunications, Beijing 102101, China*
[5]*State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai 200050, China*

*Correspondence: liu_gang@bupt.edu.cn; quheruge@bupt.edu.cn; photon.bupt@gmail.com

Abstract

First-principles calculations were carried out to predict the stability, electronic, and hydrogen passivation properties of PdS_2 nanoribbons (PdS_2NRs) with either zigzag- or armchair-terminated edges. Based the energy analysis, we reveal that the armchair NRs are more stable than the zigzag ones. Bare zigzag PdS_2NRs are metallic, irrespective of the ribbon width. On the other hand, bare armchair NRs change from metal to semiconductor when the ribbon width is greater than 1.24 nm. In addition, different hydrogen passivation type in the armchair direction leads to distinct electronic and magnetic properties of the PdS_2NRs.

Keywords: First-principles, PdS_2NRs, Hydrogen passivation, Structural properties