

# Author's Accepted Manuscript

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PII: S0921-4526(17)30641-5  
DOI: <http://dx.doi.org/10.1016/j.physb.2017.09.055>  
Reference: PHYSB310281

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 11 July 2017  
Revised date: 22 August 2017  
Accepted date: 14 September 2017

Cite this article as: Victor V. Ilyasov, Khang D. Pham, Tatiana P. Zhdanova, Huynh V. Phuc, Nguyen N. Hieu and Chuong V. Nguyen, First-principles study of structure, electronic properties and stability of tungsten adsorption on TiC(111) surface with disordered vacancies, *Physica B: Physics of Condensed Matter*, <http://dx.doi.org/10.1016/j.physb.2017.09.055>

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# First-principles study of structure, electronic properties and stability of tungsten adsorption on TiC(111) surface with disordered vacancies

Victor V. Ilyasov <sup>a</sup>, Khang D. Pham <sup>a</sup>, Tatiana P. Zhdanova <sup>a</sup>,  
Huynh V. Phuc <sup>b</sup>, Nguyen N. Hieu <sup>c</sup>, Chuong V. Nguyen <sup>c,d,\*</sup>

<sup>a</sup>*Department of Physics, Don State Technical University, Rostov on Don, Russia*

<sup>b</sup>*Division of Theoretical Physics, Dong Thap University, Dong Thap, Viet Nam*

<sup>c</sup>*Institute of Research and Development, Duy Tan University, Da Nang, Viet Nam*

<sup>d</sup>*Department of Materials Science and Engineering, Faculty of Mechanical Engineering,  
Le Quy Don Technical University, Ha Noi, Viet Nam*

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## Abstract

In this paper, we systematically investigate the atomic structure, electronic and thermodynamic properties of adsorbed W atoms on the polar Ti-terminated  $Ti_xC_y(111)$  surface with different configurations of adsorptions using first principle calculations. The bond length, adsorption energy, and formation energy for different reconstructions of the atomic structure of the  $W/Ti_xC_y(111)$  systems were established. The effect of the tungsten coverage on the electronic structure and the adsorption mechanism of tungsten atom on the  $Ti_xC_y(111)$  are also investigated. We also suggest the possible mechanisms of W nucleation on the  $Ti_xC_y(111)$  surface. The effective charges on W atoms and nearest-neighbor atoms in the examined reconstructions were identified. Additionally, we have established the charge transfer from titanium atom to tungsten and carbon atoms which determine by the re-

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