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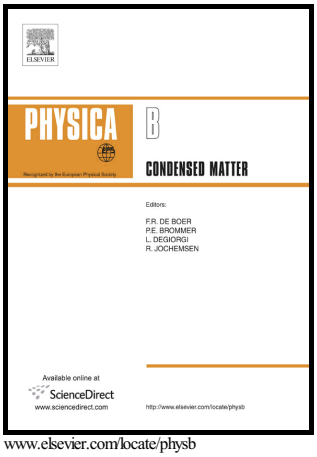

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First-principles study of structure, electronic properties and stability of tungsten adsorption on TiC(111) surface with disordered vacancies

Victor V. Ilyasov [a], Khang D. Pham [a], Tatiana P. Zhdanova [a], Huynh V. Phuc [b], Nguyen N. Hieu [c], Chuong V. Nguyen [c,d,*]

[a] *Department of Physics, Don State Technical University, Rostov on Don, Russia*

[b] *Division of Theoretical Physics, Dong Thap University, Dong Thap, Viet Nam*

[c] *Institute of Research and Development, Duy Tan University, Da Nang, Viet Nam*

[d] *Department of Materials Science and Engineering, Faculty of Mechanical Engineering, Le Quy Don Technical University, Ha Noi, Viet Nam*

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-