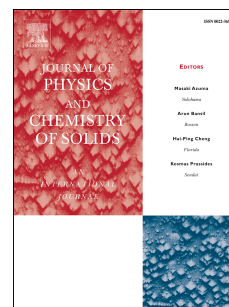


Accepted Manuscript

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PII: S0022-3697(18)30430-X

DOI: [10.1016/j.jpcs.2018.05.034](https://doi.org/10.1016/j.jpcs.2018.05.034)

Reference: PCS 8597

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 22 February 2018

Revised Date: 24 May 2018

Accepted Date: 24 May 2018

Please cite this article as: Y. Li, C. Mao, Y. Wu, Y. Shi, L. Xue, H. Li, Y. Hu, First principles study of the physical properties of $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) van der Waals heterojunctions, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.05.034.

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First principles study of the physical properties of $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) van der Waals heterojunctions

Yingying Li ^{a,1}, Caixia Mao ^{b,1}, Yunyi Wu ^c, Yifan Shi ^b, Li Xue ^b, Huailin Li ^a,
Yonghong Hu ^{a, b,*}

^a*Division of nuclear material and fuel, State Power Investment Corporation Research Institute, Beijing 100029, PR China*

^b*School of Nuclear Technology and Chemistry & Biology, Hubei University of Science and Technology, Xianning 437100, PR China*

^c*Department of Energy Materials and Technology, General Research Institute for Nonferrous Metals, Beijing 100029, PR China*

ABSTRACT

In this study, we investigated the electronic, elastic, and thermal properties of $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) van der Waals heterojunction materials using first principles calculations. The electronic properties were analyzed based on the band structure, electronic density of states, and Mulliken distribution, which showed that both materials exhibit metallic, covalent, and ionic properties. The elastic properties and mechanical stability of $\text{Ti}_3\text{SiC}_2/\text{Zr}$ and $\text{Ti}_3\text{AlC}_2/\text{Zr}$ heterostructures were also studied, and both exhibit good mechanical stability and they are ductile materials. The anisotropy results for $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) are lower than those for Zr and Ti_3AC_2 ($\text{A} = \text{Si}, \text{Al}$). The Young's modulus values for $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) are greater than those for Zr and less than those for Ti_3AC_2 ($\text{A} = \text{Si}, \text{Al}$). Furthermore, the thermal properties were analyzed based on the phonon velocity and Debye temperature, where the results showed that the thermal conductivity of $\text{Ti}_3\text{SiC}_2/\text{Zr}$ is larger than that of $\text{Ti}_3\text{AlC}_2/\text{Zr}$. The Debye temperatures decrease for the $\text{Ti}_3\text{AC}_2/\text{Zr}$ ($\text{A} = \text{Si}, \text{Al}$) van der Waals heterojunction materials as the Zr component increases.

¹ These authors contributed equally.

*Corresponding author. E-mail addresses: hchyh2001@tom.com (Y. Hu)

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