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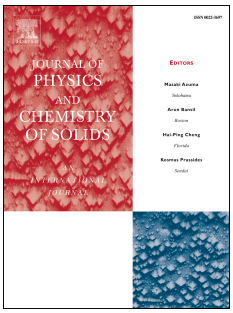

First principles study of the physical properties of Ti_3AC_2/Zr (A = Si, Al) van der Waals heterojunctions

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First principles study of the physical properties of Ti_3AC_2/Zr (A = Si, Al) van der Waals heterojunctions

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ABSTRACT

In this study, we investigated the electronic, elastic, and thermal properties of Ti_3AC_2/Zr (A=Si, 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 Ti_3SiC_2/Zr and Ti_3AlC_2/Zr heterostructures were also studied, and both exhibit good mechanical stability and they are ductile materials. The anisotropy results for Ti_3AC_2/Zr (A = Si, Al) are lower than those for Zr and Ti_3AC_2 (A = Si, Al). The Young's modulus values for Ti_3AC_2/Zr (A = Si, Al) are greater than those for Zr and less than those for Ti_3AC_2 (A = Si, Al). Furthermore, the thermal properties were analyzed based on the phonon velocity and Debye temperature, where the results showed that the thermal conductivity of Ti_3SiC_2/Zr is larger than that of Ti_3AlC_2/Zr. The Debye temperatures decrease for the Ti_3AC_2/Zr (A = Si, Al) van der Waals heterojunction materials as the Zr component increases.

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