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Mechanical properties and electronic structure of Ta₄AlC₃¹

SONGYOU WANG, MING XU, GANG YIN, LIANGYAO CHEN, State Key Laboratory of Advanced Photonic Materials and Devices, Department Optical Science and Engineering, Fudan University, Shanghai 200433, China, FENGCHUAN CHUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, YU JIA, School of Physics and Engineering, Zhengzhou University, Zhengzhou 450052, China — The mechanical properties and electronic structure of Ta₄AlC₃ have been studied using the first-principles calculations. Optimized structural parameters of the crystal structure and the calculated bulk modulus are in good agreement with the experimental data. The calculated bulk modulus reaches up to 262.40 GPa, which is the largest among all the known materials with MAX phases in the literature, the band-structure and the density of states suggest that Ta₄AlC₃ is metallic. Further analysis shows that the alternating stacks of relatively strong Ta-C bonding and weak Ta-Al bonding lead to the large bulk modulus of Ta₄AlC₃, but softening in shear.

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