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Structural and electronic properties of MXene phase of Mo2C under external stresses

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Mxene is a group of 2D materials known for their promising properties for industrial electronic devices and gas sensing behavior. The objective of this study is to investigate the electronic property of a MXene named dimolybdenum carbide (Mo_2C) under applying biaxial stress and our problem is how will the material change when biaxial stress is applied. All the possible phases have been atomistically optimized by using GGA-PBE functional with energy cut-off 650 eV, in order to verify the thermodynamic stability. It is found that the most stable phase is $P\bar{3}m1$ (Mo_2C) with lattice parameters of a = 3.054 Å and c = 4.656 Å. The $P\bar{3}m1$ phase has been cleaved to be the MXene structure and investigated for the relative properties. The biaxial stress has been reversely calculated with optimized atomic configuration of fixed biaxial stain varied up to 45%. The finding shows that Mo_2C is a non-magnetic material which is in good agreement with previous calculation. By applying biaxial strain, the stress-strain relation indicates that elastic limit is at strain of 15%. The MXene structure is formed by ionic bonding between 2p-C and 4d-Mo states. We can conclude that there are certain changes from normal in this material when applying biaxial stress. For further work, the electronic property will be carefully interpreted, as well as the superconductive behavior of this MXene when under biaxial stress will be carried out.

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