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**PROCEEDINGS**

# Tension, Shear and Bending Properties of Two-Dimensional Materials

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**ABSTRACT**

Due to excellent physical performance and potential application in the nanoscale fluid channel, 2D transition-metal dioxides and dichalcogenides with 1H phase are of great interest. Their mechanical property attracts much attention but the accurate evaluation still faces challenges because of the ultrasoft and ultrathin structure. In this work, we establish an analytical atom-based molecular mechanics model to predict the elastic modulus, Poisson's ratio and shear modulus of the single-layer 2D transition-metal dioxides and dichalcogenides. The proposed method is validated through the calculation of the mechanical property of Molybdenum disulfide ($MoS_2$). The results indicate that the elastic modulus, Poisson's ratio and shear modulus of $MoS_2$ with infinite size are 178.9 GPa, 0.22 and 73.3 GPa, respectively [1]. We can observe the obvious dependence of the elastic modulus, Poisson's ratio and shear modulus on the chiral direction and characteristic size. Based on the constructed analytical method, we report a library composed of the mechanical properties of 34 types of 1H-$MX_2$. It is found that the mechanical performances of 1H-$MX_2$ depend on the period and group numbers of elements. The obtained results are in good agreement with the existing experimental and numerical results. Furthermore, the roles of molecular structure and force field on the mechanical properties are revealed, which is beneficial in predicting the mechanical performances of the potential and unreported 1H-$MX_2$. For the bending stiffness, a coaxial spring-driven method is established, which exhibits great ability in the computation of the bending behavior for the ultrasoft two-dimensional materials [2,3]. The findings offer an important theoretical basis for the reverse design and optimization of 1H-$MX_2$ material-based nanodevices, nanochannel, etc., through nanostructure-property relationships.

**KEYWORDS**

Two dimensional materials; elastic modulus; poisson's ratio; shear modulus

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