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Stress effects on structural, elastic and electronic properties of bulk MoS_2

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The stability limit of crystalline MX_2 laminar materials under variable stress conditions is of capital interest for their technological applications. Quantum-mechanical simulations can provide useful and accurate information on this limit. In this contribution we perform first-principles density functional theory calculations to quantitatively evaluate the behavior of bulk molybdenum disulfide under general stress conditions. We show the anisotropy of the crystalline structure along principal crystallographic directions and the Van Der Walls nature of the inter-layer forces, we determine a complete, consistent set of accurate values for lattice and elastic constants. We also elucidate the change in material properties that occur when hydrostatic pressure (HP), normal compression (NC), biaxial tensile (BT) and biaxial compression (BC) are applied. The compression ratio, the transition from semiconductor to semi metal, the pressure dependence of the elastic constants and the nature (direct versus indirect) of the band gap are discussed. Deformation potentials that quantify these changes are reported. The good agreement with experiments for small strain validates our methodology and our calculated values.

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