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Equilibrium and elastic properties of hexagonal molybdenum disulphide

Equilibrium and elastic properties of hexagonal molybdenum disulphide (MoS2) are investigated using the full-potential all electrons linearised augmented plane wave method. Generalized gradient approximation of Perdew-Burke-Ernzerhof for solids (GGA_PBE_Sol) was chosen to calculate equilibrium electronic structure and elastic properties. Electronic band structure and density of states results suggest a semiconductor material with an indirect narrow energy band gap. Elastic constants C11, C12, C13, C33, and C44, bulk modulus (Bo), shear modulus (G), Young's modulus (Y), and Bo/G ratio in the same symmetry were also calculated at 0 GPa. All acquired results were compared with related experimental and theoretical data.

Keywords: Molybdenum disulphide, band gap, equilibrium structure, electronic band structure, density of states, elastic properties.

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