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Equilibrium and elastic properties of hexagonal molybdenum disulphide

Equilibrium and elastic properties of hexagonal molybdenum disulphide (MoS_2) 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 C_{11} , C_{12} , C_{13} , C_{33} , and C_{44} , bulk modulus (B_0), shear modulus (G), Young's modulus (Y), and B_0/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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Primary authors: Dr MAHLADISA, Mokete Abram (University of Limpopo); MCDONALD, Tshepho

Co-authors: Dr NTSENDWANA, Bulelwa (Mintek); Prof. SIKHWIVHULU, Lucky (Mintek); Dr MATSHABA, Malil (University of Limpopo); Prof. MOSUANG, Thuto (university of limpopo)

Presenter: MCDONALD, Tshepho

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