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Ab initio calculation of structural and electronic properties of 3c-Silicon Carbide: Density functional calculations

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Silicon Carbide has become one of the promising materials that can be used for electronic and optical applications. This is as a result of its superior properties among them structural, thermal, chemical,electronic and mechanical. This material is among the prominent systems that exhibits several polytypism. It has more than 200 polytypes and among them is 3C polytype which has attracted more
attention due to its favorable electronic properties. SiC is used in microelectronic devices such as high-power and high-temperature applications. However, a deep understanding of the physical properties of SiC is necessary due to technological problems that need to be addressed before the material can be
used in the production of electronic devices. This work reports both the structural such as bond length, lattice parameter and electronic properties of cubic Silicon Carbide (3C). The theoretical calculations were carried out using Ab initio approach based on Density Functional Theory framework within
Generalized Gradient Approximation using Perdew, Burke and Ernzerhof exchange correlation functional using Ultrasoft pseudopotential as implemented in Quantum ESPRESSO computer code. The lattice parameter was found to be overestimated by +0.66% when compared to the experimental value of 8.24 bohr while the bulk modulus was underestimated by 11.25%. The band structure was determined using Γ, X, W K, L, W Γ high symmetry points. Cubic Silicon Carbide was found to have an indirect band gap of 1.34 eV between X and Γ which is underestimated by the Density Functional Theory calculations. The system exhibit a small band gap indicating it is a semiconductor necessary in technological and industrial applications.

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