Investigation of structural and electron properties of CO2MnSi using density functional theory

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Abstract Today, widely used structural and electron properties of materials such as semi-metals have been studied experimentally. Semi-metals are ferromagnetic materials that behave like metal in a spin-like direction like metal and in the other direction of spin. Meanwhile, Haweslar Alloys are among the materials predicted by empirical calculations for their semi-metallic property. The main objective of this thesis is to study the structural and electron-specific properties of the C02MnSi Haweslar alloy. The work is based on the method of density functional theory, which is one of the strongest methods for solving a N electron device. In the C02MnSi Alloy Hollow Alloys, structural and electron calculations have been performed using the Studio Materials Software, and the results obtained with the help of approximations derived LDA, GGA, and LDA U have also been compared with the experimental results. In this case, the electron density density diagram The approximation of the LDA U in the low-spin state created a band gap, which is very close to the empirical value, indicating the semi-metallic property of the C02MnSi alloy.

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