عنوان مقاله:

A Theoretical Investigation for Electronics Structure of Mg(Bio2)2 Semiconductor Using First Principle Approach

محل انتشار:

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خلاصه مقاله:

The Mg(BiO2)2 is the orthorhombic crystal system acting as semiconductor in electric devices. To evaluate electronic band structures, the total density of state (TDOS) and the partial density of state (PDOS), Generalized Gradient Approximation (GGA) based on the Perdew–Burke–Ernzerhof (PBE0) was used for Mg(BiO2)2. The band gap was recorded at 0.959 eV, which is supported by a good semiconductor. The density of states and partial density of states were simulated for evaluating the nature of 5s, 4d for Mg, 6s, 4f, 5d, 6p for Bi and 2s, 2p for O atom for Mg(BiO2)2 to explain the transition of the electron due to hybridization. From the PDOS, it was illustrated that the d orbital of Bi .atom responses for conducting the electronic holes

کلمات کلیدی:

Electronic band structures, TDOS, PDOS, GGA and Mg(BiO2)2