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Study of Structural and Electronic Properties of Intercalated Transition Metal Dichalcogenides Compound $MTiS_2$ (M=Cr, Mn, Fe) by Density Functional Theory

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ABSTRACT

In the present work, we have studied intercalated transition metal dichalcogenides (TMDC) compound $MTiS_2$ compound (M = Cr, Mn, Fe) by Density Functional Theory (DFT) with Generalized Gradient Approximation (GGA). We have computed the structural and electronic properties by using First principle method in QUANTUM ESPRESSO computational package with an ultra-soft pseudopotential. A guest 3d transition metal M (Cr, Mn, Fe) can be easily intercalated in pure transition metal dichalcogenides compound TiS_2. In the present work, the structural optimization, electronic properties like the energy band structure, density of states (DoS), partial or projected density of states (PDoS) and total density of states (TDoS) are calculated. From the energy band structure of $MTiS_2$ compound has been overlapped energy band in the Fermi region. We conclude that the TiS_2 intercalated compound has a small band gap while the doped compound with guest 3d – atom has metallic behavior as shown from its overlapped band structure.

Keywords: Density Functional Theory (DFT), Generalized Gradient Approximation (GGA), Quantum ESPRESSO code, Intercalated compound, Transition metal dichalcogenide (TMDC).