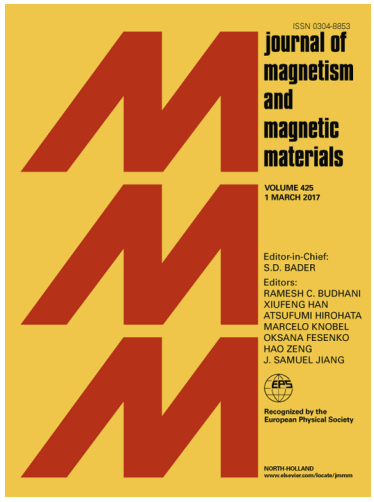

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Prediction of half-metallic properties in $TlCrS_2$ and $TlCrSe_2$ based on density functional theory

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ABSTRACT

Half-metallic properties of $TlCrS_2$, $TlCrSe_2$ and hypothetical TlCrSSe have been investigated by first-principles all-electron full-potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method based on density functional theory (DFT). The results of calculations show that $TlCrS_2$ and TlCrSSe are half-metals with energy gap (E_g) ~0.12 ev for spin-down channel. Strong hybridization of p-state of chalchogen and d-state of Cr leads to bonding and antibonding states and subsequently to the appearance of a gap in spin-down channel of $TlCrS_2$ and TlCrSSe. In the case of $TlCrSe_2$, there is a partial hybridization and p-state is partially present in the DOS at Fermi level making this compound nearly half- metallic. The present calculations revealed that total magnetic moment keeps its integer value on a relatively wide range of changes in volume (-10% ÷ 10%) for $TlCrS_2$ and TlCrSSe, while total magnetic moment of $TlCrSe_2$ decreases with increasing volume approaching to integer value 3μB.

Keywords: First-principles calculations, Half-metallic properties, spintronics

1. Introduction

Searching for new half-metallic materials with 100% spin polarization is an actual problem of material science in connection with the future development of spintronics as an alternative to the electronics. Because of the experimental difficulties to establish half-metallicity, the main method searching for new half-metallic ferromagnetic materials nowadays are electronic structure calculations [1]. We assume that the compound $TlCrS_2$ and $TlCrSe_2$, which according to [2,3] are ferromagnetic, may exhibit the half-metallic ferromagnetic properties. The integer total magnetic moments can be accounted using Slater-Pauling rule modified by Kübler [4]. In the semiconductor compounds $A^{III}B^{III}C_2^{VI}$ eighteen electrons completely fill nine valence bands. Thus, the number of occupied bands in semiconducting channel of $TlCrS_2$ is nine. The total number of electron/unit-cell is twenty one and from the Slater-Pauling rule the total magnetic moment of $TlCrS_2$ should be 3 μB/unit-cell.