

HIGH SPIN POLARIZATION IN FULL HEUSLER CO₂MNZ (Z = SI, GA, GE, SN) ALLOYS

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The full Co-based Heusler alloys are of particular interest because among them there can be found half-metallic ferromagnets (HMF), spin gapless semiconductors (SGS) [1], or topological semimetals (TSM) [2]. In our work, we carried out first-principles calculations of Co₂MnZ alloys for Z= Si, Ga, Ge, Sn on the basis of density functional theory (DFT), the exchange-correlation functional was chosen in the form of GGA PBE. And study the electronic structure, magnetic properties and spin polarization in the selected Co₂MnZ alloys. It was found that the Co₂MnGa alloy has the lowest spin polarization value about 51% and a total magnetic moment about 4.2 μ_B . For Z = Ge, Si and Sn, there is an increase of the total magnetic moment up to 5 μ_B . In the case of Co₂MnSn, the value of the total moment is equal to 5.1 μ_B – the largest among all the studied alloys. Co₂MnGe and Co₂MnSi have the highest spin polarization at the Fermi level, 92 and 99%, respectively, Co₂MnSn has 65% spin polarization. From these results, Co₂MnGe, Co₂MnSi and Co₂MnSn alloys are half-metallic ferromagnets and have potential for use in spintronics devices. This research was supported by Russian Science Foundation RSF # 22-42-02021.

References

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