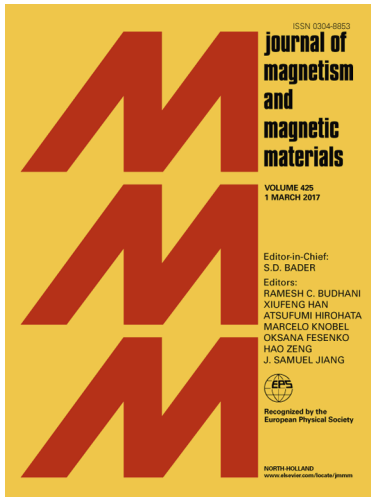

Research articles

Electronic Structure, Magnetic and Optical properties of Co_2TiZ (Z=B, Al, Ga, In) Heusler alloys

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Electronic Structure, Magnetic and Optical properties of Co_2TiZ (Z=B, Al, Ga, In) Heusler alloys

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Abstract. Electronic structure, magnetic and optical properties of Co_2TiZ (Z=B, Al, Ga, In) Heusler alloys have been computed by density functional theory implemented in WIEN2k within generalized gradient approximation for exchange correlation functions. Lattices constants, bulk modulii, energy gaps, spin polarization and density of states have been calculated. Negative value of formation energy of these alloys evidences their stability. Spin polarization of Co_2TiZ (Z=Al, B, Ga, In) are 100%, 99%, 97% and 80% respectively and Co_2TiAl shows true half metallic ferromagnetism. Co_2TiZ, for Z=B, Al, Ga, shows stable half metallically over a wide range of pressure making them suitable for fabricating thin films for spintronics applications. Optical parameters such as complex dielectric function, refractive index, reflectivity, absorption, extinction coefficient, optical conductivity have also been calculated.

Keywords: Heusler alloy, Electronic structure properties, half metallicity, Spintronics, Magnetism, Optical properties.