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Electronic structure properties of new equiatomic CoCuMnZ (Z=In, Sn, Sb) quaternary Heusler alloys: an ab-initio study

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Abstract: The electronic structure, elastic, magnetic and exchange coupling properties of new equiatomic quaternary Heusler alloys CoCuMnZ (for Z= In, Sn, Sb) have been studied using the full-potential linear muffin-tin orbital method. Total energy calculations show that formation of these alloys are energetically favorable and that they are stable in the ferromagnetic phase. Total density of states establish that CoCuMnIn and CoCuMnSn possess metallic behavior at equilibrium lattice constant and show half metallicity on lattice compression. CoCuMnSb is a true half metallic at the equilibrium lattice constants with an indirect band gap of ~0.5 eV. The calculated values of elastic constants show that CoCuMnIn/Sn also have mechanical stability. In CoCuMnZ, Co-Mn, Mn-Mn and Mn-Co couple ferromagnetically resulting in high Curie temperature in these alloys.

Keywords: Quaternary Heusler Alloys, Electronic Structure Calculation, Half Metallic Ferromagnetism, Magnetic Properties, Exchange Coupling, Elastic Properties.