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First Principles Study of a New Half-Metallic Ferrimagnets Mn2–Based Full Heusler Compounds: Mn2ZrSi and Mn2ZrGe

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Abstract : Half-metallic properties of new predicted Mn2-based full Heusler alloys Mn2ZrSi and Mn2ZrGe have been studied by first-principles full-potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method based on density functional theory (DFT). Our investigation is focused on the structural, elastic, electronic and magnetic properties of these compounds. The AlCu2Mn-type structure is found to be energetically more favorable than the CuHg2Ti-type structure for both compounds and are half-metallic ferrimagnets (HMFIs) with total magnetic moments of 2.000 µB per formula unit, well consistent with Slater-Pauling rule (Mtot = (24 – Ztot) µB). Calculations show that both the alloys have an indirect band gaps, in the majority-spin channel, with values of 0.505 eV and 0.278 eV for Mn2ZrSi and Mn2ZrGe, respectively. It was found that Mn2ZrSi and Mn2ZrGe preserved their half-metallicity for lattice constants range of 5.85–6.38 Å and 6.05–6.38 Å, respectively, and kept a 100% of spin polarization at the Fermi level. Moreover, the calculated formation energies and elastic constants confirm that these compounds are stable chemically and mechanically, and the good crystallographic compatibility with the lattice of semiconductors used industrially makes them promising magnetic materials in spintronic applications.

Keywords : first-principles calculations, full Heusler structure, half-metallic ferrimagnets, elastic properties
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