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Half-metallic characteristic in the new full-Heusler $SrYO_2$ (Y = Sc, Ti, V and Cr) *

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Half-metallic properties of $SrYO_2$ (Y = Sc, Ti, V, and Cr) full-Hensler compounds were studied using full-potential linearized augmented plane wave method based on density functional theory. The negative formation energies of $SrYO_2$ (Y = Sc, Ti, V, and Cr) alloys confirmed that they can be synthesized experimentally. Total energy calculations showed that $AlCu_2Mn$-type structure was the ground state structure in all compounds. In both structures, $SrYO_2$ (Y=Ti, V, and Cr) alloys were half-metallic ferrromagnets, while $SrScO_2$ was a non- magnetic metal. The origin of half-metallicity was verified for $SrCrO_2$. $SrYO_2$ (Y = Ti, V, and Cr) alloys in both structures were half-metals in a wide range of lattice constants indicating that they are quite robust against hydrostatic strains. The magnetization of $SrYO_2$ (Y = Ti, V, and Cr) alloys was mainly originated from the 3d electrons of Y(= Ti, V, and Cr) atoms and followed the Slater-Pauling rule: $M_{tot} = Z_{tot} - 12$. Generally, It is expected that $SrYO_2$ (Y = Ti, V, and Cr) alloys are promising and interesting candidates in the future spintronic field.

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