Half-metallicity of Cation modified magnetic perovskites RE2SnFeO6 (RE=Ca, Ba) from the understandings of GGA and Onsite GGA+U schemes

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May 5, 2020

Abstract

In this current investigation, DFT-based structural optimisations for understanding the cation effect on electronic-structure, phase stability, magnetism, elasto-mechanical and thermoelectric along with the thermal applicability of RE2SnFeO6 (RE=Ca, Ba) perovskites were analysed. The enhancement of band gap through the engagement of generalized gradient approximation and Hubbard method designates the half-metallic nature of these oxide perovskites. The half-metallic nature from the spectrum of band structures together with the interpretation from density of states with high spin subsystem corresponds to metallic N (Ef) ¿ 0 and in contrast to opposite-spin subsystem revails semiconducting N (Ef) = 0. The ferromagnetic unit cell magnetic moment is 4.00 μB with the excellent take part of transition metal (Fe). Mechanical strength interms of brittle and ductile feature is characterized from Pugh's ratio (B/G), Cauchy's discrepancy (C'=C12-C44) etc. Apart from this, to forecast the possible turnout of the Seebeck coefficients, electrical and lattice thermal conductivities were calculated, which directly hints these materials towards energy harvesting technologies. The overall study creates a better possibility to display a significant momentum in unlocking various spin electronic applications.

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